



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 11:57 AM EST

PDB ID : 1C1D
Title : L-PHENYLALANINE DEHYDROGENASE STRUCTURE IN TERNARY
COMPLEX WITH NADH AND L-PHENYLALANINE
Authors : Vanhooke, J.L.; Thoden, J.B.
Deposited on : 1999-07-21
Resolution : 1.25 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**
buster-report : 1.1.7 (2018)
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

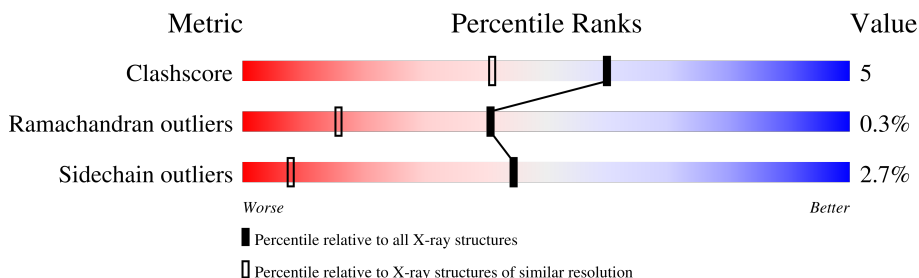
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1060 (1.28-1.24)
Ramachandran outliers	138981	1029 (1.28-1.24)
Sidechain outliers	138945	1028 (1.28-1.24)

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	355	
2	B	355	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6119 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 L-PHENYLALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2530	1562	448	508	12	0	5	0

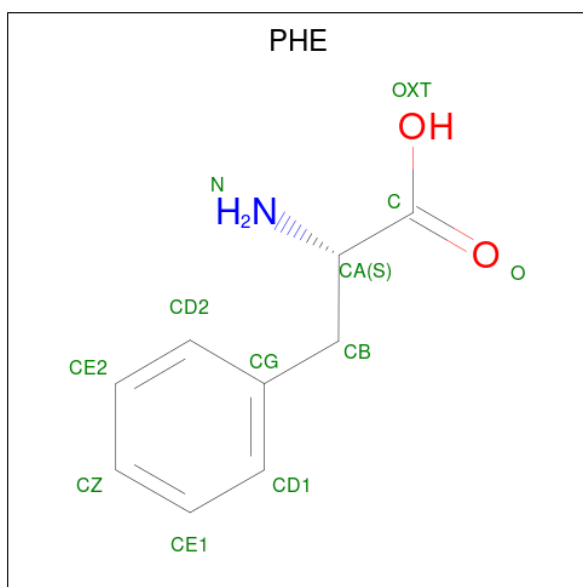
- Molecule 2 is a protein called L-PHENYLALANINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	348	2534	1565	447	510	12	0	9	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

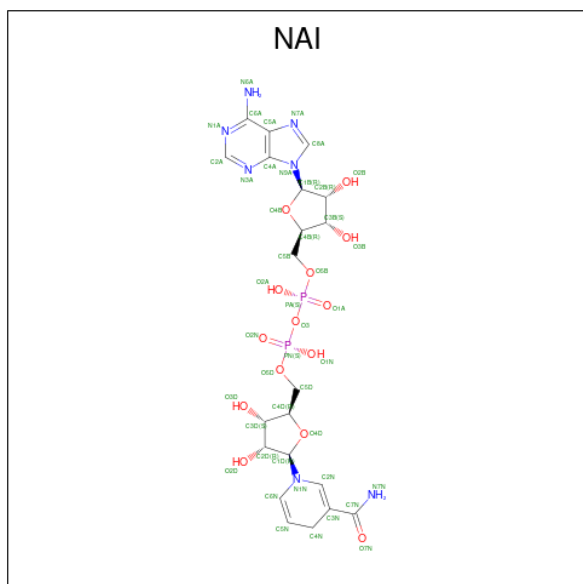
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	B	2	Total	K	0	0
			2	2		

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			12	9	1	2		
4	B	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

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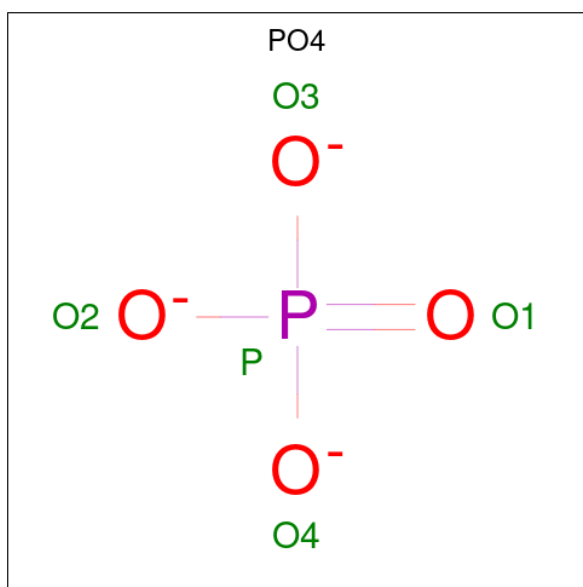
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	44	21	7	14	2	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

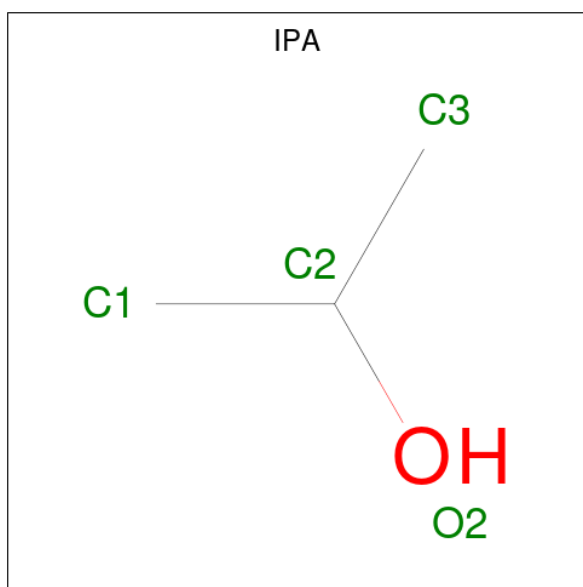
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	B	2	2	2	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
7	B	1	5	4	1	0	0

- Molecule 8 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C O 4 3 1	0	0

- Molecule 9 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	448	Total O 448 448	0	0
9	B	480	Total O 480 480	0	0

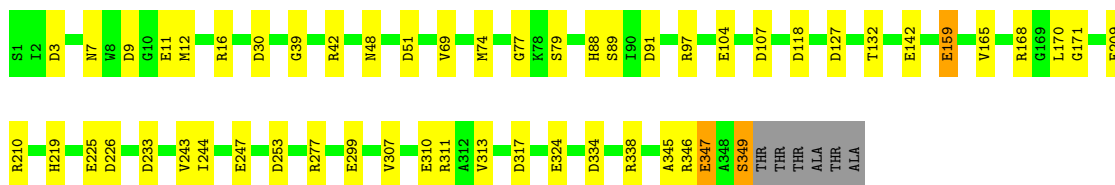
3 Residue-property plots [i](#)

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.

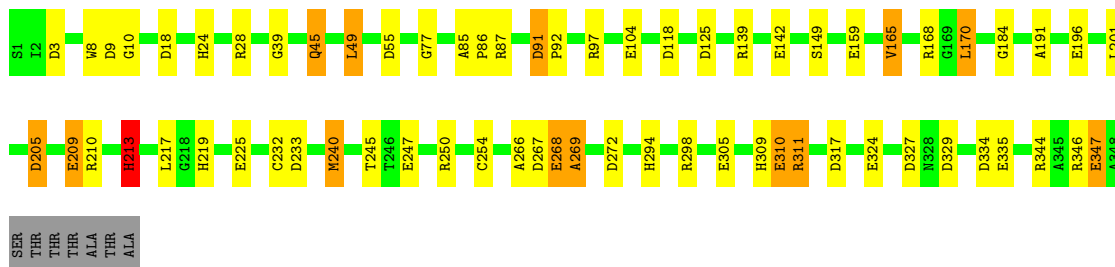
- Molecule 1: L-PHENYLALANINE DEHYDROGENASE

Chain A:  83% 14%



- Molecule 2: L-PHENYLALANINE DEHYDROGENASE

Chain B:  79% 15%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.80Å 110.60Å 113.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.25	Depositor
% Data completeness (in resolution range)	96.0 (30.00-1.25)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5E	Depositor
R, R_{free}	0.193 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6119	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, NA, K, PO4, IPA

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	0.96	13/2590 (0.5%)	1.42	37/3527 (1.0%)
2	B	0.97	11/2610 (0.4%)	1.45	37/3554 (1.0%)
All	All	0.96	24/5200 (0.5%)	1.43	74/7081 (1.0%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	104	GLU	CD-OE2	7.91	1.34	1.25
1	A	104	GLU	CD-OE2	7.46	1.33	1.25
2	B	305	GLU	CD-OE2	6.82	1.33	1.25
1	A	324	GLU	CD-OE2	6.67	1.32	1.25
1	A	299	GLU	CD-OE2	6.36	1.32	1.25
2	B	310	GLU	CD-OE2	6.09	1.32	1.25
1	A	142	GLU	CD-OE2	6.05	1.32	1.25
2	B	196	GLU	CD-OE2	6.04	1.32	1.25
1	A	225	GLU	CD-OE2	6.04	1.32	1.25
1	A	11	GLU	CD-OE2	5.83	1.32	1.25
1	A	159	GLU	CD-OE2	5.80	1.32	1.25
1	A	247[A]	GLU	CD-OE2	5.78	1.32	1.25
1	A	247[B]	GLU	CD-OE2	5.78	1.32	1.25
2	B	159	GLU	CD-OE2	5.74	1.31	1.25
2	B	324	GLU	CD-OE2	5.65	1.31	1.25
2	B	268	GLU	CD-OE2	5.59	1.31	1.25
1	A	310	GLU	CD-OE2	5.56	1.31	1.25
2	B	347	GLU	CD-OE2	5.45	1.31	1.25
2	B	142	GLU	CD-OE2	5.34	1.31	1.25
1	A	347[A]	GLU	CD-OE2	5.25	1.31	1.25
1	A	347[B]	GLU	CD-OE2	5.25	1.31	1.25
1	A	209	GLU	CD-OE2	5.18	1.31	1.25
2	B	209	GLU	CD-OE2	5.14	1.31	1.25
2	B	225	GLU	CD-OE2	5.01	1.31	1.25

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	ARG	NE-CZ-NH2	-14.40	113.10	120.30
2	B	97	ARG	NE-CZ-NH2	-10.81	114.89	120.30
2	B	267	ASP	CB-CG-OD1	10.63	127.86	118.30
2	B	267	ASP	CB-CG-OD2	-10.07	109.24	118.30
1	A	168	ARG	NE-CZ-NH2	-9.93	115.33	120.30
2	B	205	ASP	CB-CG-OD1	9.90	127.21	118.30
2	B	210	ARG	NE-CZ-NH1	9.86	125.23	120.30
2	B	311	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	91	ASP	CB-CG-OD2	-9.47	109.77	118.30
1	A	338	ARG	NE-CZ-NH1	8.86	124.73	120.30
2	B	344	ARG	NE-CZ-NH2	-8.70	115.95	120.30
2	B	97	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	317	ASP	CB-CG-OD1	8.32	125.79	118.30
1	A	127	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	42	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	16	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	118	ASP	CB-CG-OD1	7.71	125.24	118.30
2	B	272	ASP	CB-CG-OD1	7.60	125.14	118.30
2	B	298	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	B	205	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	A	317	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	A	253	ASP	CB-CG-OD1	7.44	124.99	118.30
1	A	30	ASP	CB-CG-OD2	-7.31	111.72	118.30
2	B	213	HIS	CA-CB-CG	7.19	125.83	113.60
2	B	317	ASP	CB-CG-OD1	7.02	124.62	118.30
2	B	3	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	89	SER	N-CA-CB	-6.75	100.37	110.50
2	B	344	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	A	97	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	B	233	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	B	28	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	51	ASP	CB-CG-OD1	6.54	124.19	118.30
2	B	18	ASP	CB-CG-OD1	6.51	124.16	118.30
2	B	118	ASP	CB-CG-OD1	6.47	124.12	118.30
2	B	9	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	253	ASP	CB-CG-OD2	-6.42	112.52	118.30
2	B	18	ASP	CB-CG-OD2	-6.38	112.55	118.30
1	A	107	ASP	CB-CG-OD1	6.35	124.01	118.30
2	B	250	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	346	ARG	NE-CZ-NH2	-6.21	117.20	120.30
2	B	165	VAL	CA-CB-CG1	6.08	120.02	110.90
2	B	268	GLU	N-CA-CB	6.06	121.50	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	B	91	ASP	CB-CG-OD2	-5.95	112.94	118.30
2	B	327	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	74[A]	MET	CG-SD-CE	5.86	109.58	100.20
1	A	74[B]	MET	CG-SD-CE	5.86	109.58	100.20
1	A	210	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	334	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	91	ASP	CB-CG-OD1	5.83	123.55	118.30
2	B	139	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	277	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	9	ASP	CB-CG-OD2	-5.60	113.26	118.30
2	B	87	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	3	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	B	346	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	B	334	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	347[A]	GLU	CB-CA-C	5.45	121.30	110.40
1	A	347[B]	GLU	CB-CA-C	5.45	121.30	110.40
1	A	51	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	168	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	233	ASP	CB-CG-OD1	5.41	123.17	118.30
2	B	269	ALA	N-CA-CB	5.41	117.67	110.10
2	B	125	ASP	CB-CG-OD2	-5.33	113.51	118.30
2	B	329	ASP	CB-CG-OD2	-5.28	113.55	118.30
2	B	118	ASP	N-CA-CB	5.24	120.02	110.60
1	A	97	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	B	91	ASP	CB-CG-OD1	5.18	122.97	118.30
2	B	329	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	233	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	B	311	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	226	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	219	HIS	CA-CB-CG	-5.03	105.06	113.60
1	A	12	MET	CG-SD-CE	-5.01	92.18	100.20

There are no chirality outliers.

There are no planarity outliers.

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	2530	0	2474	12	0
2	B	2534	0	2478	35	1
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	12	0	8	0	0
4	B	12	0	8	0	0
5	A	44	0	27	0	0
5	B	44	0	27	3	0
6	B	2	0	0	0	0
7	B	5	0	0	0	0
8	B	4	0	8	0	0
9	A	448	0	0	4	0
9	B	480	0	0	8	1
All	All	6119	0	5030	47	1

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 5.

All (47) 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)
2:B:311:ARG:HG3	2:B:311:ARG:HH11	1.42	0.81
2:B:209:GLU:HB2	9:B:1724:HOH:O	1.87	0.74
2:B:309:HIS:HB3	9:B:1854:HOH:O	1.88	0.73
2:B:335:GLU:HG3	9:B:1509:HOH:O	1.90	0.72
2:B:24:HIS:CG	2:B:49:LEU:HD21	2.28	0.69
1:A:243:VAL:HG23	1:A:244:ILE:HG13	1.75	0.66
2:B:240:MET:HB2	9:B:1518:HOH:O	1.95	0.64
1:A:311:ARG:HD3	9:A:1973:HOH:O	1.98	0.62
2:B:168:ARG:HG3	2:B:170[B]:LEU:HD21	1.84	0.59
2:B:45:GLN:HG2	9:B:1902:HOH:O	2.04	0.57
2:B:55[B]:ASP:OD1	9:B:1911:HOH:O	2.17	0.56
2:B:201:LEU:HD22	2:B:219:HIS:CE1	2.42	0.55
2:B:85:ALA:HB1	2:B:86:PRO:HD2	1.89	0.54
2:B:168:ARG:HG3	2:B:170[B]:LEU:CD2	2.37	0.54
2:B:168:ARG:HB3	2:B:170[B]:LEU:HD23	1.90	0.53
2:B:39:GLY:HA3	2:B:77:GLY:O	2.10	0.51
2:B:91:ASP:HB2	2:B:92:PRO:HD2	1.93	0.50
2:B:232:CYS:O	2:B:254:CYS:HA	2.12	0.50
1:A:7:ASN:ND2	9:A:1372:HOH:O	2.29	0.49
2:B:311:ARG:HH11	2:B:311:ARG:CG	2.19	0.49
1:A:39:GLY:HA3	1:A:77:GLY:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLU:HG3	1:A:313:VAL:HA	1.94	0.49
2:B:268:GLU:O	9:B:1884:HOH:O	2.21	0.47
2:B:8:TRP:CH2	2:B:10:GLY:HA3	2.49	0.47
2:B:184:GLY:HA3	5:B:760:NAI:O5B	2.15	0.47
2:B:311:ARG:CG	2:B:311:ARG:NH1	2.78	0.47
2:B:245:THR:HA	2:B:266:ALA:HB3	1.98	0.46
2:B:311:ARG:HG3	2:B:311:ARG:NH1	2.18	0.45
2:B:24:HIS:CD2	2:B:49:LEU:HD21	2.51	0.45
1:A:311:ARG:NH2	9:A:1127:HOH:O	2.47	0.45
2:B:205:ASP:HA	5:B:760:NAI:N3A	2.31	0.45
1:A:345:ALA:O	1:A:349:SER:OG	2.35	0.44
2:B:191:ALA:HB1	2:B:201:LEU:CD2	2.47	0.44
2:B:149:SER:HB3	2:B:294:HIS:CD2	2.52	0.44
1:A:307:VAL:O	1:A:311:ARG:HG2	2.17	0.44
2:B:205:ASP:OD1	5:B:760:NAI:H1B	2.17	0.44
2:B:149:SER:HB3	2:B:294:HIS:HD2	1.83	0.43
1:A:165:VAL:HG12	1:A:171:GLY:O	2.18	0.42
1:A:79:SER:HB3	9:A:1764:HOH:O	2.18	0.42
2:B:85:ALA:HB1	2:B:86:PRO:CD	2.50	0.42
2:B:191:ALA:HB1	2:B:201:LEU:HD23	2.00	0.41
2:B:191:ALA:O	2:B:201:LEU:HD21	2.21	0.41
2:B:240:MET:SD	2:B:240:MET:N	2.87	0.41
2:B:213:HIS:CE1	9:B:1981:HOH:O	2.73	0.41
1:A:132:THR:O	1:A:132:THR:HG22	2.21	0.40
1:A:165:VAL:HG13	1:A:170:LEU:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:GLU:OE1	9:B:1929:HOH:O[4_556]	2.02	0.18

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	352/355 (99%)	348 (99%)	4 (1%)	0	100	100
2	B	355/355 (100%)	344 (97%)	9 (2%)	2 (1%)	25	5
All	All	707/710 (100%)	692 (98%)	13 (2%)	2 (0%)	41	16

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	347	GLU
2	B	269	ALA

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	260/259 (100%)	254 (98%)	6 (2%)	50	12
2	B	264/260 (102%)	255 (97%)	9 (3%)	37	4
All	All	524/519 (101%)	509 (97%)	15 (3%)	44	7

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	69	VAL
1	A	88	HIS
1	A	347[A]	GLU
1	A	347[B]	GLU
1	A	349	SER
2	B	45	GLN
2	B	49	LEU
2	B	165	VAL
2	B	170[A]	LEU
2	B	170[B]	LEU

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Mol	Chain	Res	Type
2	B	213	HIS
2	B	217	LEU
2	B	240	MET
2	B	310	GLU

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	71	ASN
1	A	88	HIS
1	A	167	HIS
1	A	181	GLN
1	A	200	GLN
1	A	309	HIS
2	B	45	GLN
2	B	181	GLN
2	B	200	GLN
2	B	263	ASN
2	B	294	HIS
2	B	320	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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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
5	NAI	B	760	-	42,48,48	1.17	3 (7%)	47,73,73	1.44	7 (14%)
4	PHE	B	761	-	11,12,12	0.72	0	14,15,15	2.06	5 (35%)
8	IPA	B	860	-	3,3,3	0.41	0	3,3,3	0.38	0
7	PO4	B	880	3	4,4,4	1.52	1 (25%)	6,6,6	1.03	1 (16%)
5	NAI	A	360	-	42,48,48	1.15	3 (7%)	47,73,73	1.51	5 (10%)
4	PHE	A	361	-	11,12,12	0.99	1 (9%)	14,15,15	1.48	2 (14%)

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
5	NAI	A	360	-	-	4/25/72/72	0/5/5/5
4	PHE	B	761	-	-	4/8/8/8	0/1/1/1
5	NAI	B	760	-	-	3/25/72/72	0/5/5/5
4	PHE	A	361	-	-	3/8/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	760	NAI	C2N-C3N	5.02	1.49	1.34
5	A	360	NAI	C2N-C3N	3.93	1.45	1.34
5	A	360	NAI	O4B-C1B	-3.68	1.35	1.41
5	A	360	NAI	C4A-N3A	-2.43	1.32	1.35
5	B	760	NAI	O4D-C1D	-2.30	1.36	1.42
4	A	361	PHE	O-C	2.29	1.29	1.22
5	B	760	NAI	C2A-N1A	2.09	1.37	1.33
7	B	880	PO4	P-O3	-2.04	1.48	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	360	NAI	O4B-C1B-C2B	-5.13	99.43	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	360	NAI	O7N-C7N-C3N	-4.36	112.68	120.90
5	B	760	NAI	O7N-C7N-C3N	-3.95	113.47	120.90
5	A	360	NAI	C3N-C7N-N7N	3.80	124.42	117.67
5	B	760	NAI	O4B-C1B-C2B	-3.77	101.41	106.93
4	B	761	PHE	CB-CG-CD1	3.58	128.01	120.91
4	A	361	PHE	CG-CB-CA	3.52	121.44	114.13
4	B	761	PHE	OXT-C-CA	3.46	125.16	113.38
4	B	761	PHE	CG-CB-CA	3.31	121.02	114.13
5	B	760	NAI	C3N-C7N-N7N	3.10	123.17	117.67
5	A	360	NAI	C5A-C6A-N6A	2.96	124.86	120.35
4	B	761	PHE	CB-CG-CD2	-2.83	115.28	120.91
5	A	360	NAI	O5B-C5B-C4B	-2.45	100.55	108.99
5	B	760	NAI	O4D-C1D-C2D	-2.43	101.34	106.64
4	B	761	PHE	OXT-C-O	-2.38	118.69	124.09
5	B	760	NAI	C2B-C3B-C4B	-2.13	98.50	102.64
5	B	760	NAI	C2D-C3D-C4D	-2.12	98.51	102.64
4	A	361	PHE	CB-CG-CD1	2.04	124.95	120.91
7	B	880	PO4	O2-P-O1	-2.03	103.45	110.89
5	B	760	NAI	O4D-C1D-N1N	2.02	112.00	108.06

There are no chirality outliers.

All (14) torsion outliers are listed below:

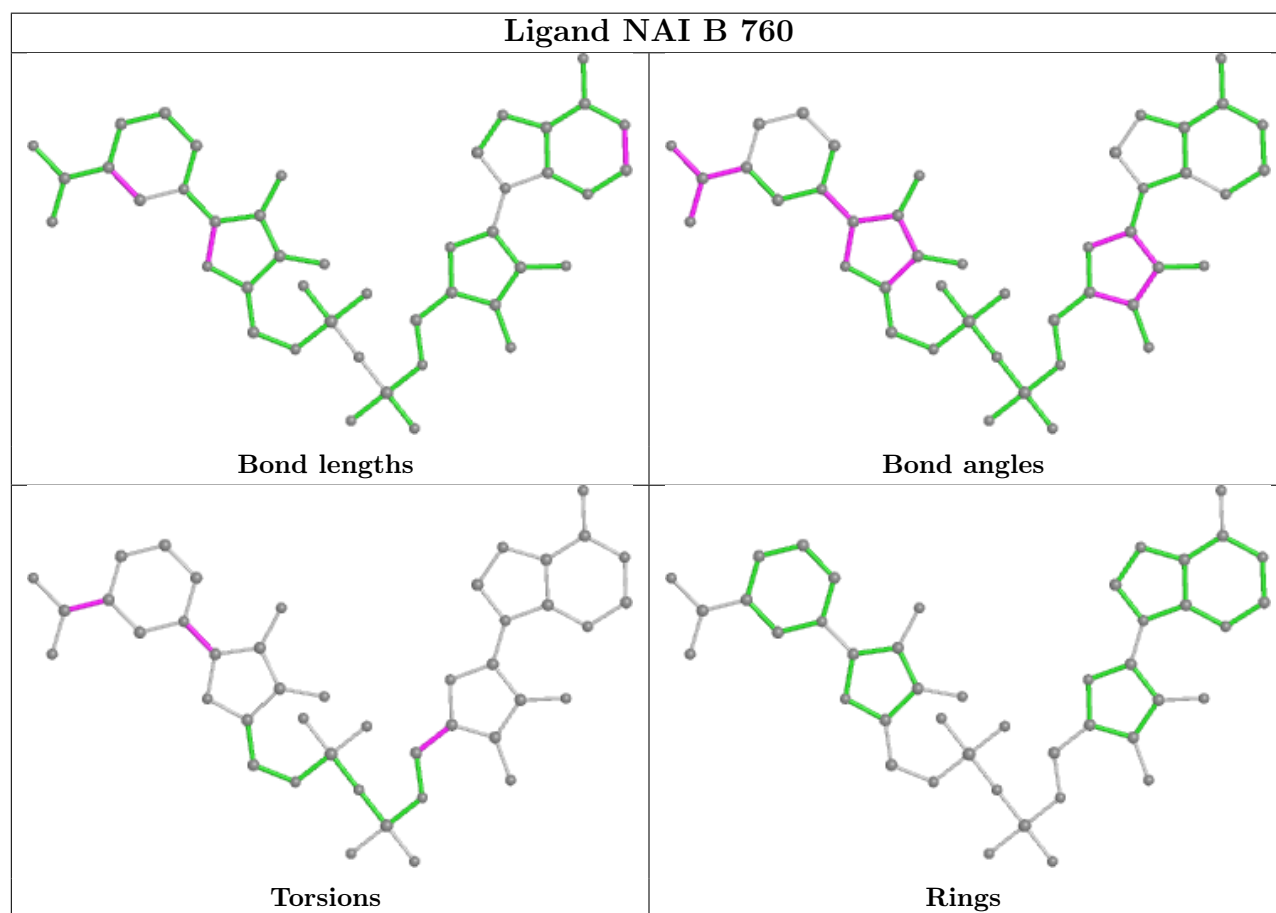
Mol	Chain	Res	Type	Atoms
4	B	761	PHE	C-CA-CB-CG
4	A	361	PHE	O-C-CA-CB
4	A	361	PHE	OXT-C-CA-CB
5	B	760	NAI	O4D-C1D-N1N-C6N
4	A	361	PHE	C-CA-CB-CG
5	A	360	NAI	O4D-C1D-N1N-C6N
4	B	761	PHE	O-C-CA-CB
4	B	761	PHE	OXT-C-CA-CB
5	B	760	NAI	O4B-C4B-C5B-O5B
5	A	360	NAI	C2D-C1D-N1N-C6N
4	B	761	PHE	OXT-C-CA-N
5	A	360	NAI	O4B-C4B-C5B-O5B
5	A	360	NAI	C2N-C3N-C7N-N7N
5	B	760	NAI	C2N-C3N-C7N-N7N

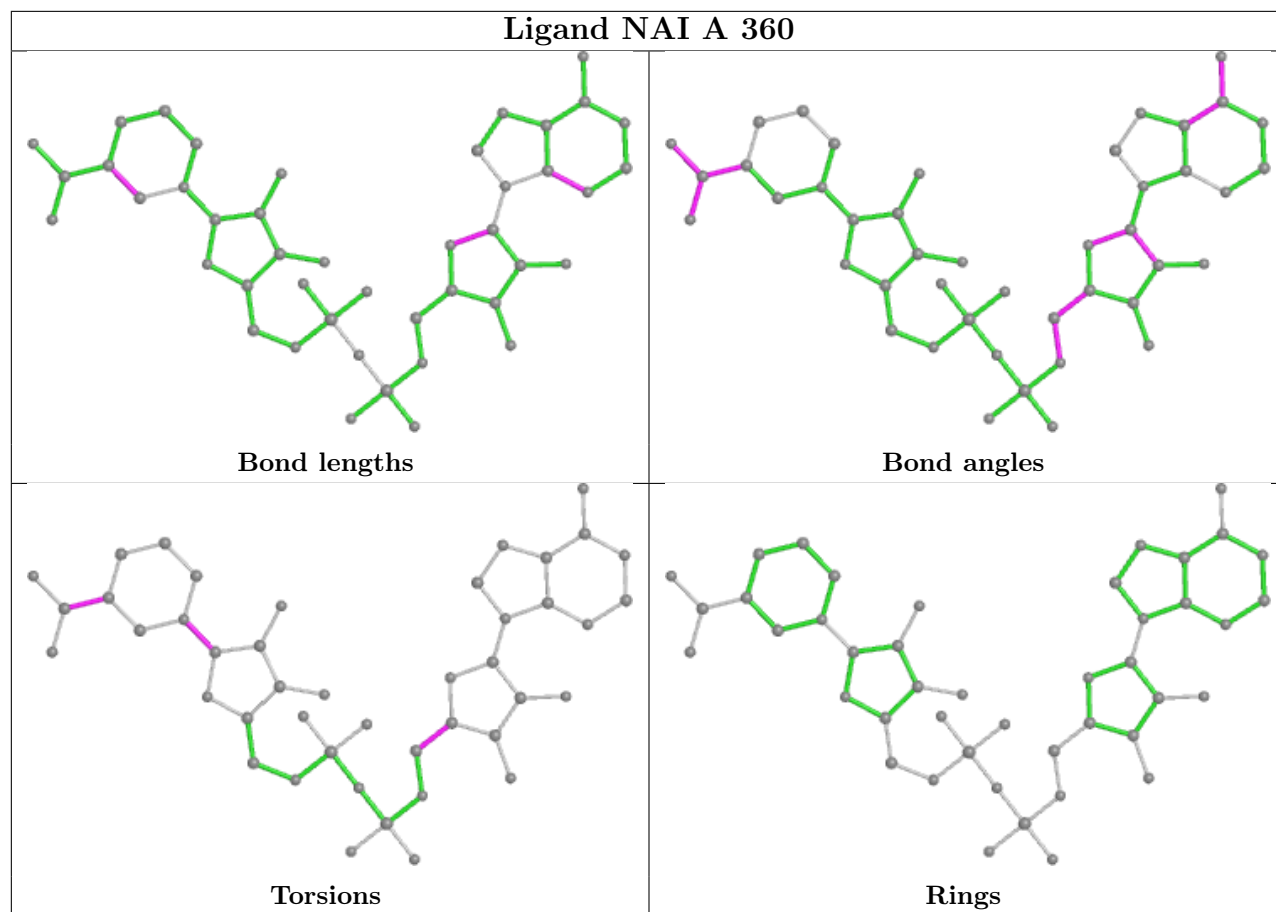
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	760	NAI	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.