



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 1ASC / pdb_00001asc
Title : THE STRUCTURAL BASIS FOR THE REDUCED ACTIVITY OF THE D223A(D222A) ACTIVE SITE MUTANT OF E. COLI ASPARTATE AMINOTRANSFERASE
Authors : Schumacher, C.; Ringe, D.
Deposited on : 1993-08-27
Resolution : 2.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

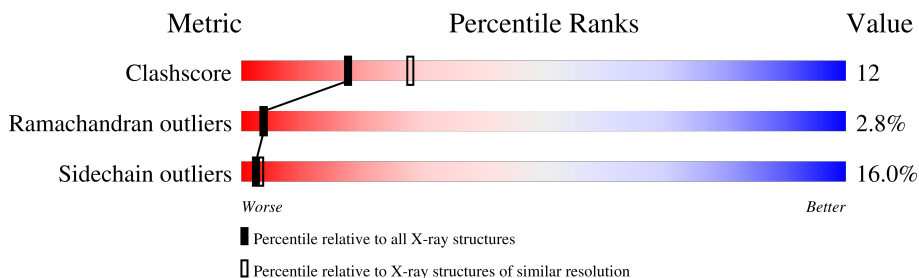
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	396	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3105 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.

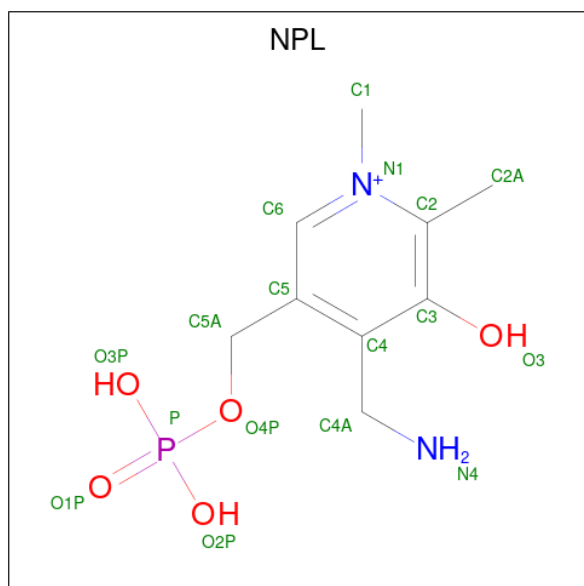
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	396	3066	1935	536	582	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	ASP	engineered mutation	UNP P00509

- Molecule 2 is N-METHYL-4-DEOXY-4-AMINO-PYRIDOXAL-5-PHOSPHATE (CCD ID: NPL) (formula: $C_9H_{16}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	17	9	2	5	1	0	0

- Molecule 3 is water.

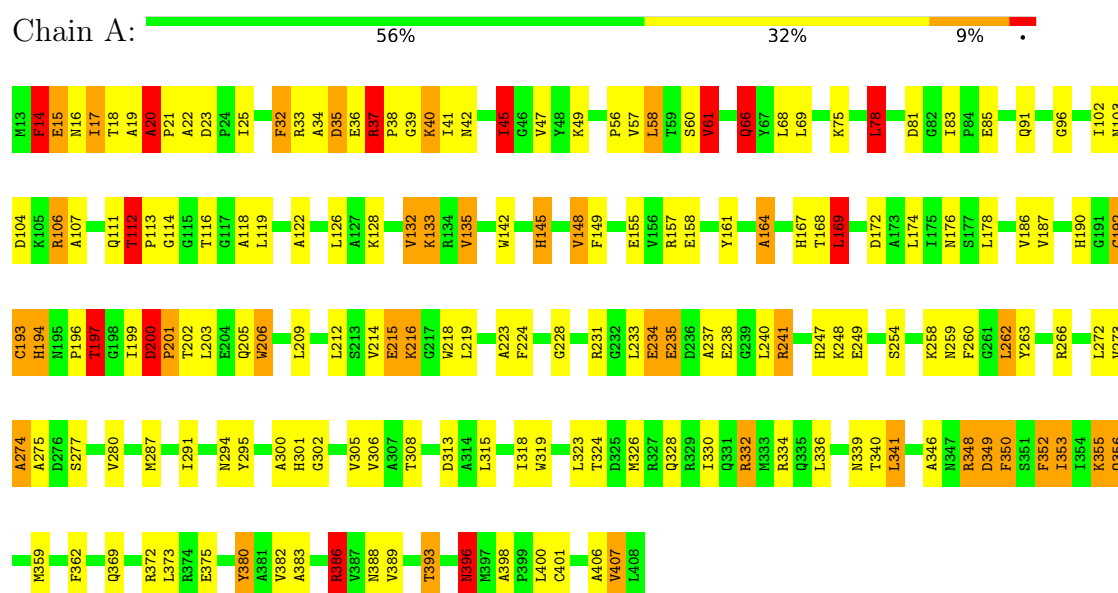
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		

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 AMINOTRANSFERASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	157.50Å 85.00Å 78.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3105	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: NPL

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	1.08	12/3127 (0.4%)	2.04	113/4236 (2.7%)

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	3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	VAL	CA-CB	8.04	1.65	1.54
1	A	190	HIS	CD2-NE2	-7.14	1.29	1.37
1	A	145	HIS	CD2-NE2	-6.69	1.30	1.37
1	A	247	HIS	CD2-NE2	-6.58	1.30	1.37
1	A	145	HIS	CG-ND1	-6.37	1.31	1.38
1	A	194	HIS	CD2-NE2	-6.30	1.30	1.37
1	A	301	HIS	CD2-NE2	-6.24	1.30	1.37
1	A	167	HIS	CD2-NE2	-5.78	1.31	1.37
1	A	25	ILE	CA-CB	5.77	1.61	1.54
1	A	190	HIS	CG-ND1	-5.68	1.32	1.38
1	A	18	THR	CA-CB	5.54	1.62	1.53
1	A	194	HIS	CG-ND1	-5.01	1.32	1.38

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	PRO	N-CA-C	12.40	130.66	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ALA	N-CA-C	11.71	127.01	110.50
1	A	197	THR	N-CA-C	11.31	124.71	111.71
1	A	18	THR	N-CA-C	-10.61	90.94	108.34
1	A	35	ASP	N-CA-C	10.47	129.57	114.39
1	A	20	ALA	N-CA-C	9.88	131.66	109.81
1	A	200	ASP	N-CA-C	9.32	130.41	109.81
1	A	20	ALA	CA-C-N	8.93	128.69	119.76
1	A	20	ALA	C-N-CA	8.93	128.69	119.76
1	A	112	THR	N-CA-CB	-8.59	95.71	111.18
1	A	356	GLN	N-CA-C	-8.53	94.33	108.32
1	A	200	ASP	O-C-N	-8.37	111.70	121.32
1	A	45	ILE	N-CA-C	-8.34	97.95	109.46
1	A	66	GLN	OE1-CD-NE2	-8.24	114.36	122.60
1	A	274	ALA	N-CA-C	7.96	126.43	114.09
1	A	18	THR	CB-CA-C	7.92	122.80	110.14
1	A	60	SER	CA-C-O	-7.76	112.33	120.55
1	A	193	CYS	N-CA-C	7.65	127.09	110.80
1	A	346	ALA	N-CA-C	7.54	120.91	110.35
1	A	32	PHE	CA-CB-CG	-7.54	106.26	113.80
1	A	33	ARG	CA-CB-CG	7.37	128.84	114.10
1	A	33	ARG	O-C-N	7.29	131.91	122.43
1	A	355	LYS	CA-C-N	7.28	134.01	121.64
1	A	355	LYS	C-N-CA	7.28	134.01	121.64
1	A	349	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	396	ASN	CA-CB-CG	7.04	119.64	112.60
1	A	112	THR	CB-CA-C	6.90	121.12	109.32
1	A	47	VAL	N-CA-C	6.89	119.02	109.45
1	A	96	GLY	CA-C-O	-6.87	117.76	122.22
1	A	112	THR	O-C-N	-6.78	117.37	121.71
1	A	193	CYS	O-C-N	6.72	131.53	122.59
1	A	66	GLN	CG-CD-NE2	6.71	126.47	116.40
1	A	200	ASP	CA-C-O	-6.64	111.07	120.16
1	A	318	ILE	N-CA-C	-6.62	104.40	110.82
1	A	32	PHE	N-CA-C	-6.57	101.50	111.56
1	A	14	PHE	N-CA-C	-6.50	104.93	112.92
1	A	407	VAL	CA-C-N	6.49	133.39	121.70
1	A	407	VAL	C-N-CA	6.49	133.39	121.70
1	A	192	CYS	CA-CB-SG	-6.46	99.54	114.40
1	A	81	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	83	ILE	CA-C-N	6.44	125.93	119.24
1	A	83	ILE	C-N-CA	6.44	125.93	119.24
1	A	20	ALA	O-C-N	-6.41	113.95	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	TRP	N-CA-C	-6.34	104.29	111.14
1	A	132	VAL	O-C-N	6.33	129.57	122.67
1	A	215	GLU	CA-CB-CG	6.32	126.74	114.10
1	A	215	GLU	N-CA-CB	-6.29	100.64	110.44
1	A	396	ASN	CB-CG-ND2	6.28	125.81	116.40
1	A	194	HIS	N-CA-C	6.25	124.12	110.80
1	A	15	GLU	O-C-N	6.21	130.85	122.59
1	A	197	THR	N-CA-CB	-6.17	100.72	110.22
1	A	355	LYS	O-C-N	6.08	130.68	122.59
1	A	193	CYS	CA-CB-SG	-6.07	100.44	114.40
1	A	190	HIS	CB-CG-CD2	-6.05	123.33	131.20
1	A	247	HIS	CA-CB-CG	-6.03	107.77	113.80
1	A	301	HIS	N-CA-C	6.03	118.38	111.02
1	A	259	ASN	CA-CB-CG	6.00	118.59	112.60
1	A	319	TRP	CG-CD2-CE3	5.99	139.89	133.90
1	A	23	ASP	CA-C-N	5.99	125.87	119.28
1	A	23	ASP	C-N-CA	5.99	125.87	119.28
1	A	353	ILE	CA-CB-CG1	-5.96	100.27	110.40
1	A	111	GLN	N-CA-C	-5.93	101.51	110.28
1	A	346	ALA	CA-C-O	5.92	127.47	121.07
1	A	294	ASN	CB-CG-ND2	5.89	125.23	116.40
1	A	122	ALA	N-CA-C	-5.84	104.83	111.14
1	A	148	VAL	N-CA-C	-5.83	104.64	110.30
1	A	330	ILE	N-CA-C	-5.81	104.85	110.42
1	A	350	PHE	CA-CB-CG	-5.75	108.05	113.80
1	A	114	GLY	CA-C-O	-5.74	117.64	122.29
1	A	262	LEU	N-CA-CB	-5.71	101.81	111.17
1	A	294	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	A	386	ARG	CB-CG-CD	-5.68	98.23	111.30
1	A	406	ALA	N-CA-C	5.68	118.24	111.71
1	A	149	PHE	CA-CB-CG	-5.68	108.12	113.80
1	A	339	ASN	CA-CB-CG	-5.67	106.94	112.60
1	A	241	ARG	CG-CD-NE	5.65	124.44	112.00
1	A	356	GLN	CB-CG-CD	5.64	122.18	112.60
1	A	372	ARG	N-CA-C	-5.62	105.23	111.36
1	A	248	LYS	N-CA-C	-5.62	105.24	111.36
1	A	187	VAL	CA-C-O	5.57	126.24	120.39
1	A	104	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	193	CYS	CA-C-O	5.55	128.44	120.51
1	A	352	PHE	CA-CB-CG	5.54	119.34	113.80
1	A	332	ARG	CA-CB-CG	5.53	125.16	114.10
1	A	339	ASN	OD1-CG-ND2	-5.53	117.07	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	THR	CA-CB-OG1	-5.52	101.32	109.60
1	A	393	THR	O-C-N	-5.51	117.25	121.55
1	A	233	LEU	N-CA-C	5.50	120.45	111.37
1	A	355	LYS	CA-C-O	5.44	128.29	120.51
1	A	396	ASN	CB-CA-C	-5.41	100.80	110.70
1	A	300	ALA	N-CA-C	5.40	117.59	111.11
1	A	238	GLU	N-CA-C	5.39	118.66	111.75
1	A	164	ALA	N-CA-CB	5.37	119.57	110.49
1	A	116	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	169	LEU	CA-C-O	-5.34	114.30	120.49
1	A	37	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	200	ASP	N-CA-CB	-5.26	101.00	110.37
1	A	214	VAL	N-CA-CB	-5.26	103.83	110.57
1	A	339	ASN	N-CA-C	5.26	116.82	111.14
1	A	61	VAL	CA-C-O	-5.25	114.58	120.25
1	A	194	HIS	CB-CG-CD2	-5.22	124.42	131.20
1	A	362	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	167	HIS	CB-CG-CD2	-5.17	124.48	131.20
1	A	234	GLU	CB-CG-CD	5.14	121.33	112.60
1	A	398	ALA	CA-C-O	-5.13	113.87	118.79
1	A	308	THR	N-CA-C	5.08	116.51	111.07
1	A	133	LYS	CG-CD-CE	5.08	122.99	111.30
1	A	193	CYS	CA-C-N	5.08	131.24	121.54
1	A	193	CYS	C-N-CA	5.08	131.24	121.54
1	A	145	HIS	CB-CG-CD2	-5.05	124.63	131.20
1	A	176	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	158	GLU	N-CA-C	5.02	116.60	108.41
1	A	78	LEU	N-CA-C	-5.02	103.77	110.55

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	ALA	Peptide
1	A	355	LYS	Mainchain
1	A	380	TYR	Sidechain

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	3066	0	3019	74	0
2	A	17	0	13	3	0
3	A	22	0	0	1	0
All	All	3105	0	3032	76	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 12.

All (76) 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:35:ASP:HB2	1:A:40:LYS:HD2	1.39	1.03
1:A:16:ASN:HB3	1:A:17:ILE:HD12	1.57	0.86
1:A:193:CYS:SG	1:A:200:ASP:HA	2.19	0.83
1:A:112:THR:HG21	1:A:118:ALA:HB2	1.61	0.81
1:A:196:PRO:HB3	1:A:386:ARG:HG3	1.68	0.76
1:A:201:PRO:HB2	1:A:205:GLN:HB2	1.69	0.74
1:A:78:LEU:HB2	3:A:513:HOH:O	1.92	0.69
1:A:197:THR:HG23	1:A:199:ILE:H	1.61	0.66
1:A:39:GLY:O	1:A:41:ILE:HG13	1.97	0.65
1:A:237:ALA:O	1:A:241:ARG:HG3	1.96	0.65
1:A:202:THR:H	1:A:205:GLN:HE21	1.43	0.65
1:A:200:ASP:HB2	1:A:201:PRO:O	1.98	0.64
1:A:192:CYS:HB2	1:A:224:PHE:CE1	2.33	0.64
2:A:409:NPL:HN41	2:A:409:NPL:H52	1.64	0.62
1:A:35:ASP:HB2	1:A:40:LYS:CD	2.22	0.60
1:A:260:PHE:HB3	1:A:262:LEU:HD22	1.83	0.60
1:A:45:ILE:HD13	1:A:49:LYS:HE2	1.84	0.60
1:A:168:THR:HG22	1:A:169:LEU:H	1.66	0.59
1:A:169:LEU:HD21	1:A:174:LEU:HD12	1.86	0.58
1:A:334:ARG:HG2	1:A:389:VAL:HG11	1.86	0.58
1:A:193:CYS:SG	1:A:200:ASP:CA	2.91	0.57
1:A:91:GLN:HE21	1:A:102:ILE:HG23	1.69	0.57
1:A:258:LYS:HD3	1:A:263:TYR:HE1	1.70	0.57
1:A:340:THR:HB	1:A:401:CYS:SG	2.45	0.57
1:A:61:VAL:HB	1:A:305:VAL:HG11	1.86	0.56
1:A:106:ARG:HH11	1:A:106:ARG:HB2	1.69	0.56
1:A:178:LEU:HB3	1:A:218:TRP:CH2	2.40	0.56
1:A:258:LYS:HG3	1:A:359:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:CB	1:A:40:LYS:HD2	2.26	0.54
1:A:277:SER:O	1:A:280:VAL:HG12	2.10	0.52
1:A:223:ALA:HB1	2:A:409:NPL:H23	1.91	0.51
1:A:91:GLN:NE2	1:A:102:ILE:HG23	2.24	0.51
1:A:228:GLY:HA3	1:A:323:LEU:HD21	1.92	0.51
1:A:348:ARG:HG3	1:A:348:ARG:HH11	1.75	0.51
1:A:369:GLN:HG2	1:A:407:VAL:HG12	1.94	0.50
1:A:194:HIS:CG	1:A:197:THR:HG22	2.47	0.49
1:A:258:LYS:HD3	1:A:263:TYR:CE1	2.47	0.49
1:A:106:ARG:O	1:A:273:VAL:HA	2.13	0.47
1:A:58:LEU:HB2	1:A:61:VAL:HG13	1.94	0.47
1:A:200:ASP:HB2	1:A:201:PRO:C	2.39	0.47
1:A:202:THR:H	1:A:205:GLN:NE2	2.12	0.47
1:A:57:VAL:HG12	1:A:61:VAL:HG22	1.98	0.46
1:A:291:ILE:HG23	1:A:295:TYR:CZ	2.51	0.46
1:A:393:THR:H	1:A:396:ASN:HB2	1.80	0.46
1:A:302:GLY:O	1:A:306:VAL:HG23	2.16	0.46
1:A:161:TYR:HE2	1:A:197:THR:HG21	1.79	0.46
1:A:142:TRP:HE3	1:A:145:HIS:CD2	2.34	0.45
1:A:359:MET:HB3	1:A:388:ASN:OD1	2.16	0.45
1:A:194:HIS:HB3	1:A:197:THR:HG22	1.99	0.45
1:A:112:THR:HG21	1:A:118:ALA:CB	2.39	0.44
1:A:323:LEU:HD12	1:A:326:MET:HE3	1.99	0.44
1:A:249:GLU:HG2	1:A:274:ALA:HA	1.98	0.44
1:A:107:ALA:HA	1:A:272:LEU:O	2.18	0.43
1:A:113:PRO:HD3	1:A:295:TYR:CZ	2.53	0.43
1:A:135:VAL:HA	1:A:186:VAL:O	2.18	0.43
1:A:194:HIS:ND1	1:A:197:THR:HG22	2.34	0.43
1:A:380:TYR:CD1	1:A:380:TYR:N	2.87	0.43
1:A:66:GLN:HE21	1:A:66:GLN:HA	1.84	0.43
1:A:266:ARG:HA	1:A:266:ARG:HD2	1.75	0.42
1:A:14:PHE:O	1:A:16:ASN:N	2.52	0.42
1:A:216:LYS:HG2	1:A:218:TRP:CZ2	2.55	0.42
1:A:42:ASN:OD1	1:A:45:ILE:HG23	2.19	0.42
1:A:224:PHE:O	1:A:254:SER:HA	2.19	0.42
1:A:39:GLY:O	1:A:40:LYS:C	2.62	0.42
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.93	0.42
1:A:35:ASP:O	1:A:37:ARG:N	2.39	0.41
2:A:409:NPL:H23	2:A:409:NPL:H11	1.85	0.41
1:A:119:LEU:HD13	1:A:145:HIS:HD2	1.85	0.41
1:A:32:PHE:CE1	1:A:40:LYS:HG2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:HG11	1:A:186:VAL:HG23	2.03	0.41
1:A:201:PRO:HD2	1:A:206:TRP:CZ2	2.56	0.41
1:A:350:PHE:O	1:A:353:ILE:HB	2.21	0.41
1:A:231:ARG:HB2	1:A:235:GLU:HB3	2.03	0.40
1:A:142:TRP:HE3	1:A:145:HIS:NE2	2.19	0.40
1:A:352:PHE:HD1	1:A:356:GLN:HE22	1.70	0.40
1:A:119:LEU:HB3	1:A:148:VAL:HG11	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	394/396 (100%)	355 (90%)	28 (7%)	11 (3%)	4 3

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA
1	A	34	ALA
1	A	164	ALA
1	A	200	ASP
1	A	19	ALA
1	A	275	ALA
1	A	383	ALA
1	A	15	GLU
1	A	40	LYS
1	A	38	PRO
1	A	17	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	319/319 (100%)	268 (84%)	51 (16%)	2 3

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	36	GLU
1	A	37	ARG
1	A	45	ILE
1	A	56	PRO
1	A	58	LEU
1	A	61	VAL
1	A	66	GLN
1	A	68	LEU
1	A	69	LEU
1	A	75	LYS
1	A	78	LEU
1	A	85	GLU
1	A	103	ASN
1	A	106	ARG
1	A	112	THR
1	A	126	LEU
1	A	128	LYS
1	A	133	LYS
1	A	135	VAL
1	A	155	GLU
1	A	157	ARG
1	A	169	LEU
1	A	172	ASP
1	A	197	THR
1	A	200	ASP
1	A	201	PRO
1	A	203	LEU
1	A	209	LEU
1	A	212	LEU

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Mol	Chain	Res	Type
1	A	215	GLU
1	A	216	LYS
1	A	219	LEU
1	A	234	GLU
1	A	235	GLU
1	A	240	LEU
1	A	287	MET
1	A	313	ASP
1	A	315	LEU
1	A	328	GLN
1	A	332	ARG
1	A	336	LEU
1	A	341	LEU
1	A	348	ARG
1	A	349	ASP
1	A	373	LEU
1	A	375	GLU
1	A	382	VAL
1	A	386	ARG
1	A	396	ASN
1	A	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	91	GLN
1	A	111	GLN
1	A	144	ASN
1	A	205	GLN
1	A	211	GLN
1	A	294	ASN
1	A	297	ASN

5.3.3 RNA ⓘ

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	NPL	A	409	-	17,17,17	1.88	6 (35%)	23,25,25	1.47	4 (17%)

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	NPL	A	409	-	-	2/8/8/8	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	409	NPL	C2A-C2	-3.22	1.43	1.49
2	A	409	NPL	C4A-C4	2.94	1.61	1.51
2	A	409	NPL	P-O3P	-2.90	1.44	1.54
2	A	409	NPL	C3-C2	-2.67	1.36	1.39
2	A	409	NPL	P-O2P	-2.66	1.44	1.54
2	A	409	NPL	C1-N1	-2.59	1.41	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	NPL	O4P-P-O1P	-4.16	95.21	106.44
2	A	409	NPL	C2A-C2-C3	-2.47	118.34	120.82
2	A	409	NPL	C2A-C2-N1	2.31	122.31	119.62
2	A	409	NPL	C4-C4A-N4	2.11	125.80	114.85

There are no chirality outliers.

All (2) torsion outliers are listed below:

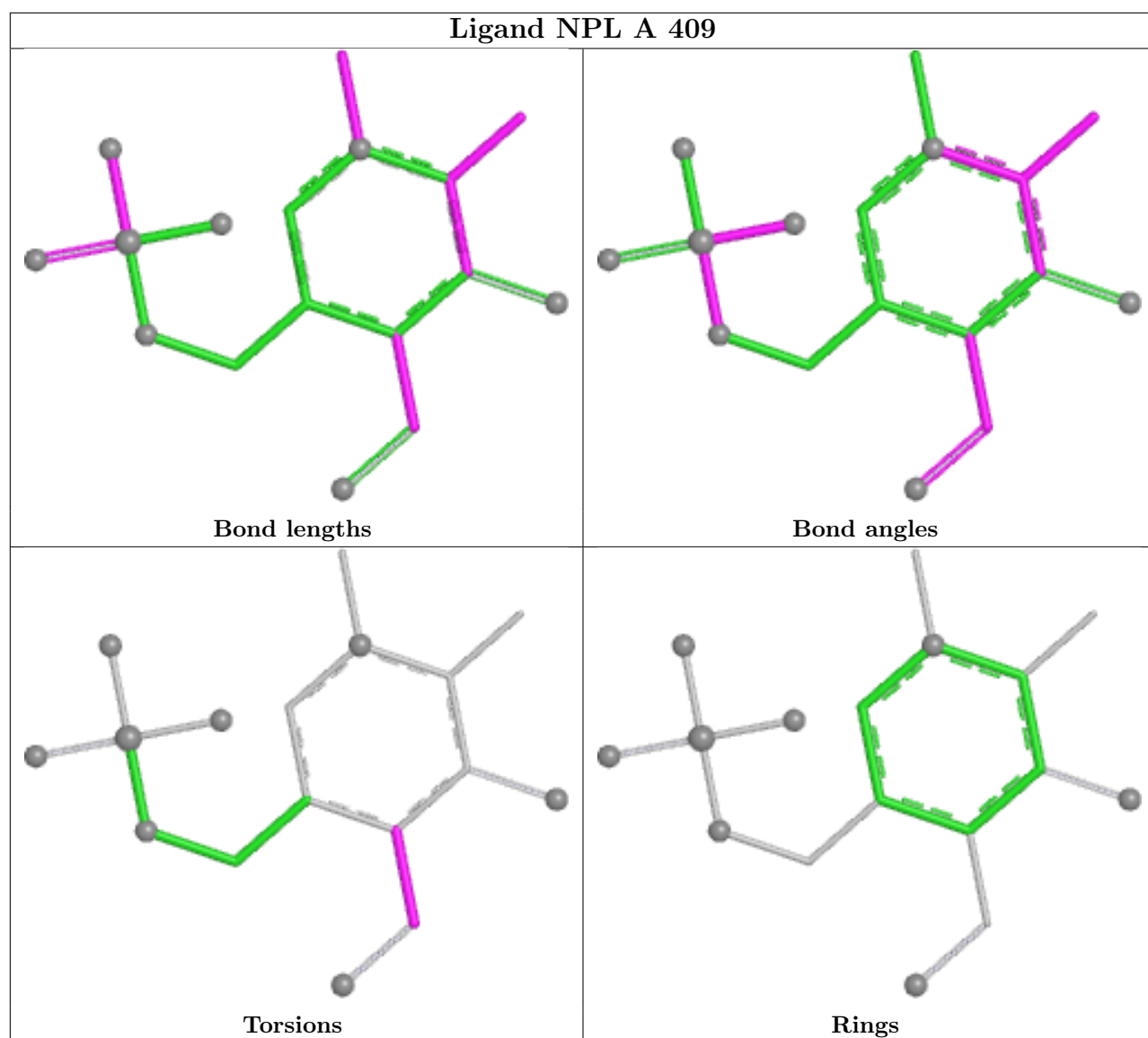
Mol	Chain	Res	Type	Atoms
2	A	409	NPL	C3-C4-C4A-N4
2	A	409	NPL	C5-C4-C4A-N4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	409	NPL	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.