



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:24 PM UTC

PDB ID : 1OXP / pdb_00001oxp
Title : ASPARTATE AMINOTRANSFERASE, H-ASP COMPLEX, CLOSED CON-
FORMATION
Authors : Hohenester, E.; Schirmer, T.; Jansonius, J.N.
Deposited on : 1995-12-23
Resolution : 2.50 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

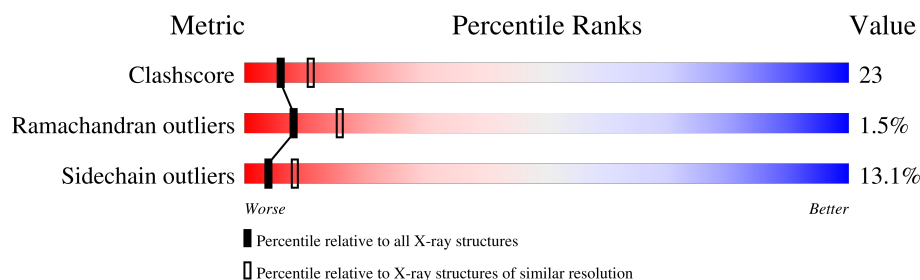
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	401	21% 47% 27% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3397 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.

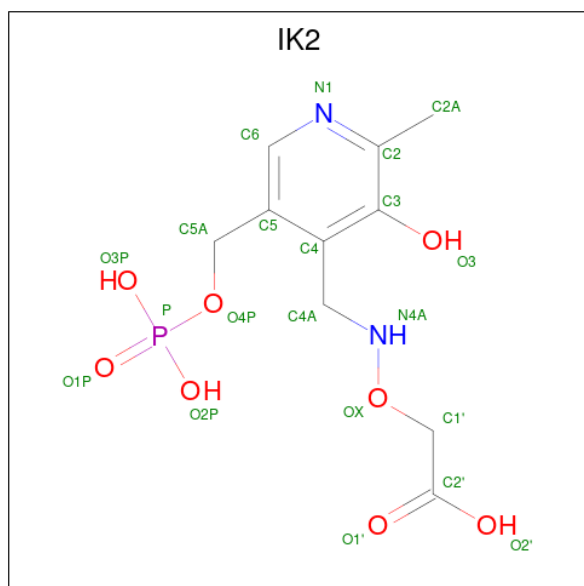
- Molecule 1 is a protein called ASPARTATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	401	3161	2004	558	581	18	5	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	PRO	SER	conflict	UNP P00508

- Molecule 2 is 4'-DEOXY-4'-ACETYLYAMINO-PYRIDOXAL-5'-PHOSPHATE (CCD ID: IK2) (formula: C₁₀H₁₅N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	21	10	2	8	1	0	0

- Molecule 3 is water.

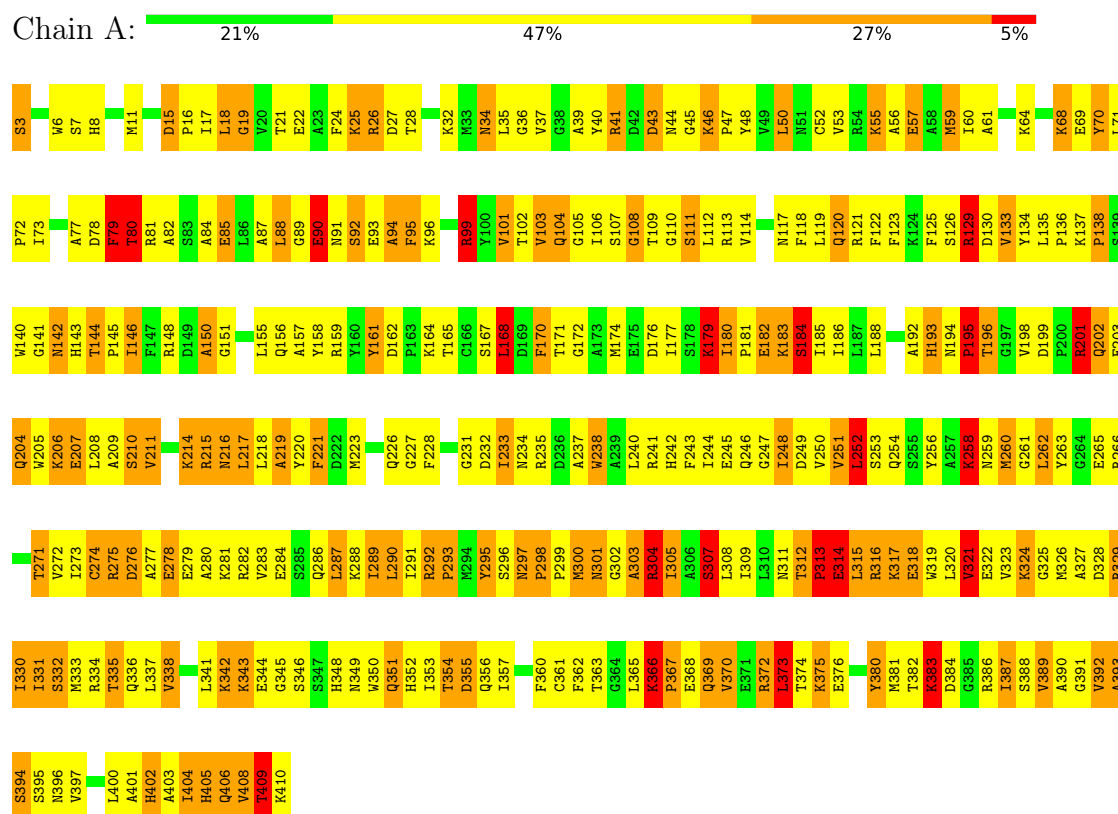
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	215	Total 215	O 215	0	0

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 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	69.50Å 91.55Å 128.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3397	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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: IK2

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	1.22	5/3231 (0.2%)	3.07	452/4360 (10.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	LYS	CA-CB	-10.63	1.36	1.53
1	A	209	ALA	C-N	-5.17	1.27	1.33
1	A	105	GLY	N-CA	5.12	1.50	1.45
1	A	361	CYS	C-N	-5.09	1.27	1.33
1	A	409	THR	CA-CB	5.08	1.62	1.54

All (452) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	ARG	CD-NE-CZ	17.80	149.32	124.40
1	A	276	ASP	CA-CB-CG	17.70	130.30	112.60
1	A	317	LYS	CA-CB-CG	13.23	140.57	114.10
1	A	202	GLN	CA-C-N	12.39	136.55	120.44
1	A	202	GLN	C-N-CA	12.39	136.55	120.44
1	A	15	ASP	CA-C-O	12.22	131.24	119.75
1	A	205	TRP	CA-C-O	-11.90	108.32	120.82
1	A	129	ARG	CD-NE-CZ	11.90	141.06	124.40
1	A	121	ARG	CA-C-O	-11.84	108.36	120.80
1	A	235	ARG	CD-NE-CZ	11.65	140.72	124.40
1	A	73	ILE	CA-C-O	-11.48	109.01	120.95
1	A	47	PRO	CB-CA-C	11.31	126.05	111.46
1	A	291	ILE	CA-C-O	-11.27	108.65	120.71
1	A	150	ALA	CA-C-N	11.21	138.21	122.29
1	A	150	ALA	C-N-CA	11.21	138.21	122.29
1	A	297	ASN	CB-CA-C	11.15	125.08	109.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ASP	CA-CB-CG	11.03	123.63	112.60
1	A	366	LYS	N-CA-CB	11.01	122.51	109.74
1	A	311	ASN	CA-CB-CG	10.85	123.45	112.60
1	A	240	LEU	CA-C-O	-10.24	110.25	121.00
1	A	284	GLU	CA-CB-CG	10.16	134.43	114.10
1	A	41	ARG	NE-CZ-NH2	-10.06	110.15	119.20
1	A	233	ILE	N-CA-C	10.02	120.84	110.62
1	A	50	LEU	CA-C-O	9.96	132.10	121.55
1	A	202	GLN	OE1-CD-NE2	9.93	132.53	122.60
1	A	125	PHE	CA-C-O	-9.79	107.81	119.27
1	A	362	PHE	CB-CA-C	9.72	126.05	111.76
1	A	196	THR	N-CA-C	9.66	123.03	111.82
1	A	249	ASP	CA-CB-CG	9.64	122.24	112.60
1	A	292	ARG	NE-CZ-NH1	-9.56	111.94	121.50
1	A	108	GLY	O-C-N	9.44	131.24	122.18
1	A	345	GLY	O-C-N	9.44	133.12	122.55
1	A	394	SER	CA-C-N	9.44	136.72	120.68
1	A	394	SER	C-N-CA	9.44	136.72	120.68
1	A	297	ASN	CA-C-N	9.42	130.09	120.38
1	A	297	ASN	C-N-CA	9.42	130.09	120.38
1	A	80	THR	CA-C-N	9.40	133.22	120.44
1	A	80	THR	C-N-CA	9.40	133.22	120.44
1	A	303	ALA	CA-C-N	9.37	133.18	120.44
1	A	303	ALA	C-N-CA	9.37	133.18	120.44
1	A	205	TRP	N-CA-CB	9.36	123.57	110.01
1	A	121	ARG	NE-CZ-NH1	9.32	130.82	121.50
1	A	256	TYR	O-C-N	9.28	133.42	122.19
1	A	375	LYS	CA-C-O	-9.25	111.17	120.70
1	A	22	GLU	CA-C-N	9.04	132.40	120.28
1	A	22	GLU	C-N-CA	9.04	132.40	120.28
1	A	406	GLN	CA-C-N	8.99	135.49	121.19
1	A	406	GLN	C-N-CA	8.99	135.49	121.19
1	A	205	TRP	N-CA-C	-8.98	101.46	111.07
1	A	373	LEU	CA-C-N	8.98	132.66	120.44
1	A	373	LEU	C-N-CA	8.98	132.66	120.44
1	A	88	LEU	N-CA-C	8.97	123.53	112.23
1	A	240	LEU	O-C-N	8.90	131.28	122.03
1	A	143	HIS	CA-C-O	-8.81	111.57	120.82
1	A	84	ALA	N-CA-C	-8.77	101.68	111.07
1	A	396	ASN	CA-CB-CG	8.77	121.37	112.60
1	A	260	MET	CA-C-O	8.74	128.67	119.05
1	A	148	ARG	CD-NE-CZ	8.71	136.59	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	HIS	N-CA-CB	8.65	122.56	110.01
1	A	325	GLY	CA-C-N	8.57	132.09	120.44
1	A	325	GLY	C-N-CA	8.57	132.09	120.44
1	A	241	ARG	NE-CZ-NH1	-8.55	112.95	121.50
1	A	304	ARG	CG-CD-NE	8.53	130.76	112.00
1	A	361	CYS	N-CA-C	-8.40	96.21	109.23
1	A	271	THR	CA-C-O	8.39	130.31	120.66
1	A	245	GLU	CB-CG-CD	8.35	126.80	112.60
1	A	315	LEU	CA-C-O	-8.27	112.19	120.70
1	A	101	VAL	O-C-N	8.21	131.48	123.03
1	A	52	CYS	CA-C-O	-8.20	110.83	120.10
1	A	171	THR	CA-CB-OG1	-8.18	97.33	109.60
1	A	241	ARG	NE-CZ-NH2	8.18	126.56	119.20
1	A	44	ASN	N-CA-C	-8.14	102.58	114.39
1	A	81	ARG	CA-C-O	-8.09	112.37	120.70
1	A	195	PRO	N-CA-C	8.08	133.12	112.10
1	A	256	TYR	CA-C-O	-8.05	109.97	119.48
1	A	125	PHE	CA-CB-CG	-8.00	105.80	113.80
1	A	408	VAL	CA-C-N	8.00	136.58	122.42
1	A	408	VAL	C-N-CA	8.00	136.58	122.42
1	A	338	VAL	CA-C-N	7.97	131.17	120.65
1	A	338	VAL	C-N-CA	7.97	131.17	120.65
1	A	117	ASN	CA-CB-CG	7.95	120.55	112.60
1	A	113	ARG	NH1-CZ-NH2	7.93	129.61	119.30
1	A	103	VAL	N-CA-CB	-7.91	100.50	111.41
1	A	148	ARG	NE-CZ-NH1	7.88	129.38	121.50
1	A	298	PRO	N-CA-C	7.85	120.27	110.70
1	A	234	ASN	OD1-CG-ND2	7.81	130.41	122.60
1	A	344	GLU	CG-CD-OE2	7.81	136.35	118.40
1	A	208	LEU	N-CA-C	-7.80	102.71	111.14
1	A	246	GLN	OE1-CD-NE2	7.80	130.40	122.60
1	A	392	VAL	N-CA-CB	-7.78	102.24	110.72
1	A	196	THR	N-CA-CB	-7.73	98.30	110.28
1	A	101	VAL	N-CA-CB	7.72	123.42	111.99
1	A	282	ARG	CA-C-N	7.72	132.90	120.55
1	A	282	ARG	C-N-CA	7.72	132.90	120.55
1	A	99	ARG	NE-CZ-NH1	-7.70	113.80	121.50
1	A	44	ASN	CA-C-O	7.67	127.51	118.69
1	A	95	PHE	CA-C-N	7.64	130.84	120.38
1	A	95	PHE	C-N-CA	7.64	130.84	120.38
1	A	209	ALA	CA-C-N	7.63	130.84	120.54
1	A	209	ALA	C-N-CA	7.63	130.84	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	143	HIS	O-C-N	7.58	129.88	122.07
1	A	180	ILE	N-CA-CB	7.57	117.12	110.08
1	A	348	HIS	CA-C-O	7.57	130.64	121.94
1	A	210	SER	CA-CB-OG	-7.56	95.98	111.10
1	A	295	TYR	CA-C-O	7.55	127.01	119.08
1	A	195	PRO	CA-C-N	7.51	131.73	120.31
1	A	195	PRO	C-N-CA	7.51	131.73	120.31
1	A	22	GLU	O-C-N	-7.49	114.06	122.08
1	A	345	GLY	CA-C-O	-7.49	110.32	118.86
1	A	286	GLN	CA-C-N	7.47	130.90	120.29
1	A	286	GLN	C-N-CA	7.47	130.90	120.29
1	A	247	GLY	O-C-N	7.47	130.79	122.50
1	A	338	VAL	CA-C-O	7.46	129.03	121.27
1	A	220	TYR	CA-C-O	7.45	128.22	120.40
1	A	151	GLY	N-CA-C	7.44	126.71	115.63
1	A	19	GLY	CA-C-O	-7.40	112.41	120.40
1	A	120	GLN	O-C-N	7.39	129.96	122.12
1	A	133	VAL	N-CA-CB	7.38	121.24	111.64
1	A	362	PHE	CA-C-N	7.38	130.91	120.28
1	A	362	PHE	C-N-CA	7.38	130.91	120.28
1	A	278	GLU	CB-CG-CD	7.38	125.14	112.60
1	A	43	ASP	CA-CB-CG	-7.37	105.23	112.60
1	A	146	ILE	N-CA-CB	7.36	119.16	110.55
1	A	81	ARG	CG-CD-NE	7.34	128.15	112.00
1	A	292	ARG	NE-CZ-NH2	7.32	125.78	119.20
1	A	25	LYS	CA-C-N	7.31	132.30	120.60
1	A	25	LYS	C-N-CA	7.31	132.30	120.60
1	A	380	TYR	CA-CB-CG	-7.30	100.75	113.90
1	A	354	THR	CA-CB-OG1	-7.30	98.65	109.60
1	A	102	THR	O-C-N	7.28	131.96	123.30
1	A	80	THR	CA-C-O	7.25	128.66	120.90
1	A	278	GLU	CA-C-O	-7.25	112.19	120.24
1	A	201	ARG	CA-C-O	-7.22	112.61	120.92
1	A	202	GLN	CG-CD-NE2	-7.21	105.59	116.40
1	A	367	PRO	N-CA-C	7.19	124.23	113.81
1	A	363	THR	O-C-N	7.14	130.58	122.22
1	A	386	ARG	NE-CZ-NH2	7.13	125.62	119.20
1	A	68	LYS	CD-CE-NZ	7.12	134.70	111.90
1	A	226	GLN	CB-CG-CD	7.10	124.67	112.60
1	A	118	PHE	CA-CB-CG	-7.08	106.72	113.80
1	A	289	ILE	CA-C-N	7.05	130.31	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ILE	C-N-CA	7.05	130.31	120.29
1	A	159	ARG	CD-NE-CZ	7.05	134.26	124.40
1	A	346	SER	CA-C-O	7.05	128.95	120.92
1	A	315	LEU	N-CA-C	-7.03	103.55	111.14
1	A	273	ILE	N-CA-CB	7.01	120.18	111.41
1	A	281	LYS	CA-C-O	-6.99	112.20	120.10
1	A	384	ASP	CA-CB-CG	6.98	119.58	112.60
1	A	73	ILE	O-C-N	6.97	128.63	121.87
1	A	318	GLU	CA-C-O	6.97	127.94	120.55
1	A	96	LYS	CA-C-N	6.95	133.31	121.14
1	A	96	LYS	C-N-CA	6.95	133.31	121.14
1	A	106	ILE	CA-C-O	6.95	129.47	120.78
1	A	184	SER	N-CA-C	-6.95	99.59	110.36
1	A	142	ASN	OD1-CG-ND2	6.94	129.54	122.60
1	A	337	LEU	CA-C-N	6.94	129.55	120.60
1	A	337	LEU	C-N-CA	6.94	129.55	120.60
1	A	60	ILE	CA-C-N	6.93	129.80	120.65
1	A	60	ILE	C-N-CA	6.93	129.80	120.65
1	A	95	PHE	O-C-N	-6.93	114.61	122.09
1	A	389	VAL	CA-C-O	6.91	128.42	119.85
1	A	301	ASN	CA-C-N	6.91	127.77	120.03
1	A	301	ASN	C-N-CA	6.91	127.77	120.03
1	A	391	GLY	N-CA-C	6.87	122.22	114.67
1	A	144	THR	CA-CB-OG1	-6.85	99.32	109.60
1	A	17	ILE	CA-C-N	6.85	129.76	120.38
1	A	17	ILE	C-N-CA	6.85	129.76	120.38
1	A	287	LEU	N-CA-C	-6.85	103.90	111.36
1	A	202	GLN	CA-C-O	6.82	130.27	120.51
1	A	22	GLU	CA-C-O	6.79	128.54	121.07
1	A	219	ALA	CA-C-N	6.78	132.97	123.07
1	A	219	ALA	C-N-CA	6.78	132.97	123.07
1	A	114	VAL	CA-C-N	6.75	127.30	119.94
1	A	114	VAL	C-N-CA	6.75	127.30	119.94
1	A	300	MET	N-CA-C	6.75	119.47	111.71
1	A	204	GLN	OE1-CD-NE2	6.75	129.35	122.60
1	A	363	THR	N-CA-C	6.75	119.47	111.71
1	A	80	THR	CA-CB-CG2	6.72	121.93	110.50
1	A	146	ILE	CB-CA-C	-6.71	103.38	111.97
1	A	176	ASP	CA-CB-CG	-6.71	105.89	112.60
1	A	11	MET	O-C-N	6.67	131.78	122.77
1	A	60	ILE	CA-C-O	6.66	127.91	120.85
1	A	259	ASN	CA-CB-CG	6.66	119.26	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ASP	O-C-N	6.64	129.26	122.09
1	A	134	TYR	O-C-N	6.62	130.75	123.13
1	A	334	ARG	CD-NE-CZ	6.60	133.64	124.40
1	A	130	ASP	N-CA-C	6.59	119.98	109.24
1	A	293	PRO	CA-C-N	6.59	132.63	122.42
1	A	293	PRO	C-N-CA	6.59	132.63	122.42
1	A	315	LEU	CB-CA-C	6.58	121.30	110.90
1	A	313	PRO	CA-C-N	6.56	129.61	120.29
1	A	313	PRO	C-N-CA	6.56	129.61	120.29
1	A	312	THR	CA-CB-OG1	-6.54	99.78	109.60
1	A	28	THR	CA-CB-OG1	-6.53	99.80	109.60
1	A	118	PHE	CA-C-O	6.53	127.43	120.70
1	A	380	TYR	CA-C-O	-6.52	113.12	120.43
1	A	238	TRP	N-CA-CB	6.52	121.51	110.49
1	A	369	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	72	PRO	N-CA-CB	6.49	109.49	103.39
1	A	305	ILE	CA-C-N	6.48	129.28	120.54
1	A	305	ILE	C-N-CA	6.48	129.28	120.54
1	A	47	PRO	N-CA-C	-6.47	101.05	111.14
1	A	146	ILE	O-C-N	6.46	128.25	121.91
1	A	111	SER	CA-C-O	6.44	127.58	120.82
1	A	363	THR	CA-C-O	-6.43	112.83	120.10
1	A	176	ASP	N-CA-C	-6.43	104.20	111.14
1	A	227	GLY	O-C-N	6.43	129.84	122.38
1	A	265	GLU	CA-C-O	6.42	126.79	119.27
1	A	374	THR	CA-C-O	6.42	127.32	120.70
1	A	19	GLY	N-CA-C	-6.40	104.86	113.24
1	A	360	PHE	CA-C-O	6.38	130.34	121.73
1	A	120	GLN	OE1-CD-NE2	-6.37	116.23	122.60
1	A	246	GLN	N-CA-C	-6.35	105.28	113.16
1	A	383	LYS	CA-CB-CG	6.35	126.80	114.10
1	A	283	VAL	CA-C-N	6.35	129.11	120.54
1	A	283	VAL	C-N-CA	6.35	129.11	120.54
1	A	388	SER	CA-C-O	6.33	127.13	120.54
1	A	278	GLU	N-CA-CB	6.33	119.63	110.20
1	A	331	ILE	N-CA-C	6.33	116.50	110.42
1	A	205	TRP	O-C-N	6.32	128.57	122.07
1	A	161	TYR	CA-CB-CG	6.30	125.25	113.90
1	A	109	THR	N-CA-CB	6.29	119.31	109.94
1	A	317	LYS	O-C-N	6.28	128.56	122.03
1	A	85	GLU	CB-CG-CD	6.28	123.27	112.60
1	A	258	LYS	N-CA-C	6.26	120.94	113.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	HIS	CB-CA-C	6.25	120.10	109.72
1	A	22	GLU	CA-CB-CG	6.25	126.60	114.10
1	A	180	ILE	O-C-N	6.24	127.93	121.07
1	A	208	LEU	O-C-N	6.22	128.81	122.09
1	A	121	ARG	CD-NE-CZ	6.21	133.09	124.40
1	A	262	LEU	CA-C-N	6.20	133.39	121.54
1	A	262	LEU	C-N-CA	6.20	133.39	121.54
1	A	280	ALA	N-CA-C	-6.20	103.67	111.11
1	A	87	ALA	CA-C-N	6.19	131.20	120.68
1	A	87	ALA	C-N-CA	6.19	131.20	120.68
1	A	256	TYR	N-CA-C	-6.19	104.22	112.94
1	A	282	ARG	CD-NE-CZ	6.18	133.06	124.40
1	A	156	GLN	OE1-CD-NE2	-6.18	116.42	122.60
1	A	302	GLY	CA-C-N	6.18	128.56	120.28
1	A	302	GLY	C-N-CA	6.18	128.56	120.28
1	A	329	ARG	CA-C-O	-6.18	114.00	120.55
1	A	182	GLU	O-C-N	-6.18	115.71	123.12
1	A	349	ASN	CA-C-O	-6.15	114.00	120.58
1	A	89	GLY	N-CA-C	-6.14	105.05	112.48
1	A	104	GLN	N-CA-C	-6.11	101.23	110.28
1	A	226	GLN	CG-CD-NE2	-6.11	107.23	116.40
1	A	392	VAL	CB-CA-C	6.11	118.49	110.91
1	A	183	LYS	CA-C-O	-6.11	113.10	120.12
1	A	188	LEU	CA-C-O	-6.09	114.12	120.70
1	A	206	LYS	N-CA-C	6.09	118.71	111.71
1	A	275	ARG	NH1-CZ-NH2	6.09	127.22	119.30
1	A	57	GLU	CA-C-N	6.08	128.42	120.28
1	A	57	GLU	C-N-CA	6.08	128.42	120.28
1	A	26	ARG	N-CA-C	6.07	119.79	112.38
1	A	88	LEU	CA-C-O	-6.07	112.63	119.79
1	A	93	GLU	N-CA-CB	6.07	119.11	110.13
1	A	291	ILE	O-C-N	6.04	129.82	121.84
1	A	252	LEU	N-CA-CB	-6.03	100.31	111.52
1	A	41	ARG	NH1-CZ-NH2	6.02	127.13	119.30
1	A	122	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	284	GLU	CG-CD-OE2	6.01	132.22	118.40
1	A	395	SER	CA-CB-OG	6.01	123.12	111.10
1	A	70	TYR	CA-CB-CG	6.00	124.70	113.90
1	A	102	THR	CA-CB-CG2	5.99	120.69	110.50
1	A	143	HIS	N-CA-C	-5.99	104.66	111.07
1	A	176	ASP	CA-C-O	-5.98	114.54	120.70
1	A	307	SER	CB-CA-C	5.96	120.98	110.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	GLU	CA-C-N	5.96	130.04	122.00
1	A	344	GLU	C-N-CA	5.96	130.04	122.00
1	A	329	ARG	NE-CZ-NH2	-5.95	113.84	119.20
1	A	218	LEU	N-CA-CB	5.95	119.67	110.21
1	A	337	LEU	CA-C-O	5.95	127.06	120.82
1	A	73	ILE	N-CA-C	-5.95	104.55	110.62
1	A	99	ARG	CA-CB-CG	5.93	125.97	114.10
1	A	41	ARG	CA-C-O	-5.92	114.30	120.70
1	A	372	ARG	CA-C-O	5.92	126.70	120.42
1	A	288	LYS	CB-CG-CD	-5.92	97.68	111.30
1	A	61	ALA	O-C-N	5.92	128.19	122.03
1	A	258	LYS	CA-C-O	5.91	126.93	119.78
1	A	126	SER	CA-C-O	-5.90	114.61	121.10
1	A	278	GLU	CA-CB-CG	5.88	125.85	114.10
1	A	179	LYS	CA-C-O	-5.87	112.48	119.35
1	A	217	LEU	CA-C-O	-5.86	114.54	121.16
1	A	3	SER	CA-C-N	5.84	132.99	122.64
1	A	3	SER	C-N-CA	5.84	132.99	122.64
1	A	46	LYS	N-CA-C	-5.84	101.32	110.14
1	A	349	ASN	N-CA-CB	-5.84	100.92	110.21
1	A	322	GLU	CA-C-O	-5.83	112.20	119.38
1	A	93	GLU	N-CA-C	-5.83	104.29	111.40
1	A	136	PRO	CA-C-O	-5.81	114.69	121.95
1	A	203	GLU	O-C-N	5.81	128.05	122.07
1	A	81	ARG	O-C-N	5.81	128.36	122.09
1	A	59	MET	CA-C-N	5.80	128.66	120.42
1	A	59	MET	C-N-CA	5.80	128.66	120.42
1	A	34	ASN	CA-CB-CG	-5.80	106.80	112.60
1	A	193	HIS	CA-C-O	5.79	127.56	121.19
1	A	108	GLY	CA-C-O	-5.77	114.77	121.00
1	A	243	PHE	N-CA-C	5.77	117.25	111.07
1	A	110	GLY	CA-C-O	-5.76	114.82	120.75
1	A	90	GLU	N-CA-C	5.75	119.55	112.54
1	A	170	PHE	CA-C-O	-5.74	114.47	120.55
1	A	370	VAL	N-CA-C	-5.74	104.93	110.72
1	A	93	GLU	CA-C-O	-5.74	114.41	120.55
1	A	360	PHE	N-CA-C	5.74	118.21	109.95
1	A	165	THR	CA-CB-OG1	-5.72	101.01	109.60
1	A	216	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	234	ASN	N-CA-C	-5.70	105.14	111.36
1	A	56	ALA	N-CA-C	-5.69	105.07	111.28
1	A	167	SER	N-CA-C	5.69	116.06	108.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	O-C-N	5.69	129.05	122.17
1	A	79	PHE	CA-C-N	5.67	128.20	120.54
1	A	79	PHE	C-N-CA	5.67	128.20	120.54
1	A	94	ALA	CA-C-O	5.67	127.65	121.02
1	A	292	ARG	CA-C-O	5.66	123.83	118.63
1	A	207	GLU	N-CA-C	5.65	119.35	112.23
1	A	138	PRO	N-CA-CB	-5.65	96.39	102.60
1	A	129	ARG	CB-CA-C	-5.64	101.18	110.72
1	A	324	LYS	CA-CB-CG	-5.62	102.85	114.10
1	A	92	SER	CA-CB-OG	5.62	122.34	111.10
1	A	207	GLU	CA-C-O	5.62	126.42	119.79
1	A	141	GLY	CA-C-O	5.62	130.34	120.57
1	A	43	ASP	CA-C-N	5.62	130.57	121.98
1	A	43	ASP	C-N-CA	5.62	130.57	121.98
1	A	113	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	A	96	LYS	CB-CA-C	5.60	120.21	110.68
1	A	231	GLY	N-CA-C	-5.60	107.60	115.32
1	A	103	VAL	CB-CA-C	5.59	118.90	110.63
1	A	366	LYS	N-CA-C	-5.58	102.88	110.36
1	A	39	ALA	O-C-N	5.57	130.41	123.28
1	A	246	GLN	N-CA-CB	5.57	118.97	110.44
1	A	335	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	6	TRP	N-CA-C	5.56	119.60	112.26
1	A	308	LEU	O-C-N	-5.55	115.82	122.15
1	A	122	PHE	CA-C-O	-5.54	112.83	119.15
1	A	117	ASN	CB-CG-ND2	-5.54	108.10	116.40
1	A	232	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	50	LEU	CA-C-N	5.52	127.99	120.54
1	A	50	LEU	C-N-CA	5.52	127.99	120.54
1	A	261	GLY	CA-C-N	5.51	131.80	122.65
1	A	261	GLY	C-N-CA	5.51	131.80	122.65
1	A	393	ALA	O-C-N	-5.51	115.99	123.10
1	A	11	MET	CA-C-O	-5.51	114.07	120.62
1	A	117	ASN	CA-C-O	-5.50	113.30	119.79
1	A	318	GLU	CA-C-N	5.50	127.96	120.54
1	A	318	GLU	C-N-CA	5.50	127.96	120.54
1	A	26	ARG	N-CA-CB	-5.49	100.98	110.32
1	A	211	VAL	CA-C-O	-5.49	114.54	120.47
1	A	142	ASN	CB-CG-OD1	-5.48	109.83	120.80
1	A	351	GLN	CB-CG-CD	5.48	121.92	112.60
1	A	141	GLY	N-CA-C	5.46	126.11	113.18
1	A	376	GLU	CB-CA-C	-5.46	98.70	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLN	CA-C-N	5.46	130.04	122.29
1	A	226	GLN	C-N-CA	5.46	130.04	122.29
1	A	281	LYS	CB-CA-C	-5.44	100.56	110.63
1	A	276	ASP	N-CA-CB	-5.44	102.23	111.31
1	A	15	ASP	N-CA-CB	5.44	119.46	109.73
1	A	78	ASP	OD1-CG-OD2	5.43	135.94	122.90
1	A	259	ASN	CB-CA-C	5.43	121.34	109.99
1	A	237	ALA	N-CA-CB	-5.42	101.63	110.42
1	A	161	TYR	CA-C-O	5.42	128.12	121.72
1	A	342	LYS	CA-C-N	5.41	128.07	120.28
1	A	342	LYS	C-N-CA	5.41	128.07	120.28
1	A	158	TYR	CA-CB-CG	5.41	123.63	113.90
1	A	7	SER	CA-C-N	5.40	132.12	121.58
1	A	7	SER	C-N-CA	5.40	132.12	121.58
1	A	99	ARG	NH1-CZ-NH2	5.40	126.32	119.30
1	A	402	HIS	N-CA-C	5.40	117.58	111.11
1	A	316	ARG	CA-C-N	5.39	127.76	120.65
1	A	316	ARG	C-N-CA	5.39	127.76	120.65
1	A	226	GLN	CB-CA-C	5.38	118.33	110.26
1	A	402	HIS	CA-C-N	5.38	127.43	120.44
1	A	402	HIS	C-N-CA	5.38	127.43	120.44
1	A	80	THR	CB-CA-C	5.38	119.41	110.81
1	A	291	ILE	N-CA-CB	5.37	119.52	110.56
1	A	277	ALA	N-CA-C	-5.36	105.47	112.23
1	A	35	LEU	CB-CA-C	5.36	119.76	111.13
1	A	148	ARG	CA-C-O	-5.36	114.82	120.55
1	A	215	ARG	NH1-CZ-NH2	-5.36	112.34	119.30
1	A	403	ALA	N-CA-C	-5.35	105.35	111.07
1	A	355	ASP	CA-C-O	-5.34	114.84	120.55
1	A	259	ASN	CA-C-O	-5.33	112.69	119.31
1	A	404	ILE	N-CA-CB	5.33	116.79	110.55
1	A	406	GLN	CB-CG-CD	-5.33	103.53	112.60
1	A	84	ALA	O-C-N	5.32	127.55	122.07
1	A	330	ILE	O-C-N	5.32	127.03	121.87
1	A	245	GLU	O-C-N	-5.32	114.67	122.43
1	A	387	ILE	CA-CB-CG2	5.31	119.53	110.50
1	A	113	ARG	NE-CZ-NH1	-5.30	116.19	121.50
1	A	396	ASN	O-C-N	5.30	128.61	122.19
1	A	47	PRO	O-C-N	5.30	129.44	123.03
1	A	35	LEU	N-CA-C	-5.30	105.27	112.26
1	A	114	VAL	CA-C-O	5.30	126.24	120.57
1	A	64	LYS	N-CA-C	-5.29	103.99	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	PHE	N-CA-CB	5.28	117.66	110.01
1	A	389	VAL	CA-CB-CG1	5.27	119.36	110.40
1	A	104	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	A	158	TYR	CA-C-O	-5.25	115.03	120.70
1	A	89	GLY	CA-C-O	-5.25	117.68	122.24
1	A	409	THR	N-CA-CB	-5.25	103.04	110.81
1	A	397	VAL	CB-CA-C	5.24	119.22	112.14
1	A	168	LEU	O-C-N	-5.23	115.91	123.07
1	A	258	LYS	CB-CA-C	-5.22	100.95	109.56
1	A	271	THR	N-CA-C	5.22	117.95	109.24
1	A	221	PHE	CA-C-N	5.22	130.10	122.85
1	A	221	PHE	C-N-CA	5.22	130.10	122.85
1	A	395	SER	CA-C-O	-5.21	113.64	119.79
1	A	73	ILE	N-CA-CB	5.20	117.61	110.54
1	A	322	GLU	CA-C-N	5.19	129.54	121.35
1	A	322	GLU	C-N-CA	5.19	129.54	121.35
1	A	390	ALA	N-CA-C	-5.18	105.06	111.33
1	A	7	SER	O-C-N	-5.18	115.90	122.27
1	A	172	GLY	O-C-N	5.18	127.93	122.28
1	A	95	PHE	CB-CA-C	5.17	119.08	110.90
1	A	321	VAL	CB-CA-C	5.17	118.80	112.02
1	A	355	ASP	N-CA-CB	5.17	117.78	110.13
1	A	119	LEU	CA-C-N	5.15	127.44	120.38
1	A	119	LEU	C-N-CA	5.15	127.44	120.38
1	A	405	HIS	CA-CB-CG	-5.15	108.65	113.80
1	A	202	GLN	CB-CG-CD	-5.14	103.87	112.60
1	A	332	SER	N-CA-CB	5.13	117.66	110.12
1	A	409	THR	OG1-CB-CG2	5.12	119.55	109.30
1	A	43	ASP	N-CA-C	5.12	121.70	110.80
1	A	321	VAL	CA-CB-CG1	5.11	119.08	110.40
1	A	400	LEU	CB-CA-C	5.11	119.27	110.79
1	A	325	GLY	CA-C-O	-5.11	115.49	120.75
1	A	242	HIS	N-CA-C	-5.10	105.72	111.28
1	A	174	MET	CB-CA-C	5.09	119.25	110.79
1	A	344	GLU	CG-CD-OE1	-5.09	106.69	118.40
1	A	77	ALA	O-C-N	5.08	127.95	122.11
1	A	113	ARG	CA-CB-CG	5.08	124.26	114.10
1	A	395	SER	CA-C-N	-5.07	114.56	122.37
1	A	395	SER	C-N-CA	-5.07	114.56	122.37
1	A	282	ARG	NE-CZ-NH1	5.07	126.56	121.50
1	A	292	ARG	CA-CB-CG	5.07	124.23	114.10
1	A	207	GLU	CA-C-N	5.06	127.33	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLU	C-N-CA	5.06	127.33	120.44
1	A	297	ASN	CA-CB-CG	5.06	117.66	112.60
1	A	82	ALA	N-CA-CB	5.06	118.12	110.28
1	A	148	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	A	150	ALA	N-CA-CB	-5.04	102.47	110.28
1	A	228	PHE	CA-CB-CG	-5.04	108.76	113.80
1	A	245	GLU	CA-C-O	5.04	125.56	119.11
1	A	314	GLU	CA-C-O	5.04	125.76	120.42
1	A	295	TYR	CA-C-N	5.03	131.15	121.54
1	A	295	TYR	C-N-CA	5.03	131.15	121.54
1	A	283	VAL	N-CA-C	-5.03	105.52	111.00
1	A	401	ALA	O-C-N	5.02	127.45	122.08
1	A	316	ARG	CG-CD-NE	-5.02	100.96	112.00
1	A	251	VAL	N-CA-CB	5.01	119.65	111.44
1	A	382	THR	O-C-N	-5.01	117.30	122.96
1	A	195	PRO	N-CA-CB	-5.00	97.10	102.60

There are no chirality outliers.

There are no planarity outliers.

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	3161	0	3154	143	1
2	A	21	0	10	3	1
3	A	215	0	0	18	1
All	All	3397	0	3164	144	2

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 23.

All (144) 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:177:ILE:HA	1:A:180:ILE:HD12	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ILE:HD13	1:A:320:LEU:HD21	1.64	0.80
1:A:370:VAL:HG12	1:A:383:LYS:HE2	1.65	0.78
1:A:350:TRP:HB3	1:A:353:ILE:HD12	1.66	0.78
1:A:338:VAL:HG21	1:A:354:THR:HG23	1.67	0.77
1:A:133:VAL:HG13	1:A:185:ILE:HG22	1.68	0.75
1:A:215:ARG:HB2	1:A:217:LEU:HG	1.69	0.74
1:A:129:ARG:HA	1:A:129:ARG:HE	1.52	0.74
1:A:162:ASP:OD1	1:A:164:LYS:HE3	1.88	0.73
1:A:314:GLU:HA	1:A:317:LYS:HD2	1.71	0.72
1:A:71:LEU:HD13	1:A:300:MET:HE3	1.72	0.71
1:A:41:ARG:HB3	1:A:45:GLY:HA2	1.74	0.69
1:A:370:VAL:HG11	1:A:383:LYS:HA	1.75	0.68
1:A:342:LYS:HG2	3:A:518:HOH:O	1.92	0.68
1:A:312:THR:HB	1:A:315:LEU:HB2	1.75	0.68
1:A:404:ILE:O	1:A:409:THR:HB	1.93	0.68
1:A:244:ILE:HA	1:A:248:ILE:O	1.95	0.67
1:A:34:ASN:HD22	1:A:36:GLY:H	1.42	0.67
1:A:211:VAL:O	1:A:215:ARG:HG2	1.97	0.64
1:A:120:GLN:HG3	1:A:150:ALA:O	1.98	0.64
1:A:196:THR:O	1:A:356:GLN:HG2	1.98	0.64
1:A:373:LEU:HD22	1:A:408:VAL:HG11	1.79	0.63
1:A:193:HIS:ND1	1:A:196:THR:HB	2.12	0.63
1:A:211:VAL:HG22	3:A:528:HOH:O	1.99	0.62
1:A:85:GLU:HG3	1:A:95:PHE:CZ	2.34	0.62
1:A:34:ASN:ND2	1:A:36:GLY:H	1.98	0.61
1:A:94:ALA:HA	1:A:99:ARG:HD3	1.83	0.61
1:A:366:LYS:HB3	1:A:367:PRO:HD2	1.80	0.61
1:A:333:MET:HE2	1:A:336:GLN:HE22	1.66	0.61
1:A:316:ARG:NH2	3:A:542:HOH:O	2.34	0.60
1:A:179:LYS:HB2	1:A:179:LYS:NZ	2.18	0.59
1:A:111:SER:HB2	1:A:253:SER:OG	2.02	0.59
1:A:194:ASN:ND2	2:A:411:IK2:O3	2.35	0.59
1:A:210:SER:O	1:A:214:LYS:HB3	2.02	0.58
1:A:183:LYS:N	1:A:216:ASN:O	2.36	0.58
1:A:79:PHE:HA	1:A:307:SER:HB2	1.85	0.58
1:A:233:ILE:HD13	1:A:320:LEU:CD2	2.32	0.58
1:A:303:ALA:O	1:A:307:SER:HB3	2.04	0.57
1:A:91:ASN:ND2	1:A:91:ASN:H	2.03	0.57
1:A:137:LYS:HD2	1:A:157:ALA:HB1	1.86	0.57
1:A:182:GLU:O	1:A:183:LYS:HB2	2.05	0.57
1:A:91:ASN:ND2	3:A:610:HOH:O	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HD2	1:A:258:LYS:N	2.20	0.56
1:A:332:SER:O	1:A:335:THR:HB	2.06	0.55
1:A:352:HIS:HA	1:A:355:ASP:HB2	1.88	0.55
1:A:144:THR:HB	1:A:145:PRO:HD3	1.89	0.55
1:A:314:GLU:H	1:A:314:GLU:CD	2.15	0.55
1:A:333:MET:HE2	1:A:336:GLN:NE2	2.22	0.54
1:A:181:PRO:O	1:A:184:SER:OG	2.26	0.54
1:A:170:PHE:CE1	1:A:204:GLN:HB3	2.43	0.54
1:A:40:TYR:OH	1:A:329:ARG:HD3	2.07	0.54
1:A:221:PHE:O	1:A:252:LEU:HA	2.08	0.53
1:A:186:ILE:HG23	1:A:186:ILE:O	2.07	0.53
1:A:123:PHE:CD2	1:A:185:ILE:HD11	2.44	0.53
1:A:207:GLU:O	1:A:211:VAL:HG23	2.08	0.53
1:A:329:ARG:NH1	1:A:392:VAL:O	2.41	0.53
2:A:411:IK2:C4A	2:A:411:IK2:O4P	2.58	0.52
1:A:366:LYS:HB3	1:A:367:PRO:CD	2.39	0.52
1:A:312:THR:O	1:A:313:PRO:C	2.51	0.52
1:A:251:VAL:HG12	1:A:272:VAL:HG22	1.91	0.52
1:A:161:TYR:CD1	1:A:196:THR:HG23	2.44	0.52
1:A:183:LYS:HB2	3:A:554:HOH:O	2.09	0.52
1:A:356:GLN:HG3	3:A:549:HOH:O	2.11	0.51
1:A:142:ASN:O	1:A:146:ILE:HG13	2.10	0.51
1:A:333:MET:CE	1:A:336:GLN:HE22	2.22	0.51
1:A:91:ASN:H	1:A:91:ASN:HD22	1.59	0.51
1:A:34:ASN:HD22	1:A:34:ASN:C	2.19	0.51
1:A:80:THR:HG23	3:A:466:HOH:O	2.10	0.51
1:A:104:GLN:NE2	1:A:303:ALA:HB2	2.26	0.51
1:A:15:ASP:OD1	1:A:16:PRO:HD2	2.12	0.50
1:A:298:PRO:HB2	1:A:299:PRO:HD2	1.94	0.50
1:A:43:ASP:OD2	1:A:394:SER:OG	2.27	0.50
1:A:71:LEU:CD1	1:A:300:MET:HE3	2.41	0.50
1:A:292:ARG:HB3	1:A:293:PRO:HD3	1.94	0.50
1:A:55:LYS:O	1:A:59:MET:HG3	2.10	0.50
1:A:338:VAL:CG2	1:A:354:THR:HG23	2.40	0.50
1:A:373:LEU:HD23	1:A:381:MET:HE1	1.95	0.49
1:A:219:ALA:HB3	1:A:250:VAL:HG12	1.95	0.49
1:A:15:ASP:O	1:A:16:PRO:C	2.56	0.49
1:A:196:THR:HG22	1:A:198:VAL:HG23	1.95	0.49
1:A:314:GLU:CD	1:A:314:GLU:N	2.70	0.48
1:A:321:VAL:O	1:A:324:LYS:HB2	2.13	0.48
1:A:326:MET:O	1:A:330:ILE:HG13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HH12	1:A:393:ALA:HA	1.78	0.48
1:A:108:GLY:O	1:A:112:LEU:HB2	2.14	0.48
1:A:330:ILE:HG23	1:A:389:VAL:HG13	1.94	0.48
1:A:287:LEU:HA	1:A:287:LEU:HD23	1.76	0.47
1:A:368:GLU:H	1:A:368:GLU:CD	2.23	0.47
1:A:343:LYS:C	1:A:343:LYS:HD3	2.39	0.47
1:A:48:TYR:N	3:A:415:HOH:O	2.27	0.47
1:A:327:ALA:HB1	3:A:479:HOH:O	2.14	0.47
1:A:101:VAL:O	1:A:271:THR:HA	2.15	0.47
1:A:258:LYS:NZ	2:A:411:IK2:H4A2	2.30	0.46
1:A:27:ASP:HB3	1:A:32:LYS:HD3	1.98	0.46
1:A:365:LEU:HD23	1:A:369:GLN:NE2	2.31	0.46
1:A:309:ILE:HA	1:A:315:LEU:HB3	1.98	0.45
1:A:373:LEU:CD2	1:A:381:MET:HE1	2.46	0.45
1:A:69:GLU:HB3	3:A:604:HOH:O	2.16	0.45
1:A:298:PRO:CB	1:A:299:PRO:HD2	2.47	0.45
1:A:260:MET:HE2	1:A:309:ILE:HG21	1.99	0.45
1:A:8:HIS:H	1:A:8:HIS:CD2	2.34	0.44
1:A:144:THR:CB	1:A:145:PRO:HD3	2.47	0.44
1:A:223:MET:O	1:A:254:GLN:HA	2.17	0.44
1:A:18:LEU:HD12	1:A:18:LEU:HA	1.93	0.44
1:A:201:ARG:O	1:A:204:GLN:N	2.50	0.44
1:A:168:LEU:CD1	1:A:198:VAL:HG12	2.48	0.44
1:A:140:TRP:HA	3:A:560:HOH:O	2.18	0.43
1:A:290:LEU:HD21	3:A:593:HOH:O	2.17	0.43
1:A:26:ARG:NH2	3:A:452:HOH:O	2.52	0.43
1:A:137:LYS:HD2	1:A:157:ALA:CB	2.49	0.43
1:A:182:GLU:HA	1:A:215:ARG:O	2.18	0.43
1:A:53:VAL:HG13	1:A:305:ILE:HG21	2.01	0.43
1:A:357:ILE:HD12	1:A:357:ILE:O	2.18	0.43
1:A:343:LYS:HE2	3:A:488:HOH:O	2.18	0.42
1:A:387:ILE:HD13	1:A:387:ILE:HG21	1.81	0.42
1:A:338:VAL:O	1:A:341:LEU:HB2	2.19	0.42
1:A:319:TRP:O	1:A:323:VAL:HG23	2.20	0.42
1:A:372:ARG:NH2	3:A:603:HOH:O	2.52	0.42
1:A:318:GLU:HB2	3:A:583:HOH:O	2.19	0.42
1:A:324:LYS:HD2	1:A:324:LYS:HA	1.85	0.42
1:A:15:ASP:HB3	1:A:19:GLY:H	1.84	0.42
1:A:21:THR:O	1:A:25:LYS:HG3	2.20	0.42
1:A:179:LYS:HB2	1:A:179:LYS:HZ2	1.85	0.42
1:A:53:VAL:O	1:A:57:GLU:HG3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG13	1:A:185:ILE:CG2	2.43	0.42
1:A:313:PRO:HB2	1:A:314:GLU:CD	2.45	0.42
1:A:405:HIS:O	1:A:406:GLN:C	2.62	0.42
1:A:135:LEU:CD1	1:A:155:LEU:HD22	2.50	0.41
1:A:328:ASP:O	1:A:331:ILE:HB	2.20	0.41
1:A:27:ASP:OD2	1:A:380:TYR:OH	2.23	0.41
1:A:313:PRO:HB2	1:A:314:GLU:OE2	2.21	0.41
1:A:402:HIS:O	1:A:406:GLN:HG2	2.19	0.41
1:A:206:LYS:HG3	1:A:238:TRP:HH2	1.85	0.41
1:A:45:GLY:HA2	3:A:588:HOH:O	2.20	0.41
1:A:194:ASN:HA	1:A:195:PRO:HA	1.84	0.41
1:A:260:MET:HB3	1:A:262:LEU:HG	2.03	0.41
1:A:369:GLN:O	1:A:373:LEU:HB2	2.21	0.41
1:A:90:GLU:HG2	3:A:612:HOH:O	2.20	0.41
1:A:274:CYS:HB3	1:A:279:GLU:HG2	2.02	0.41
1:A:15:ASP:CG	1:A:16:PRO:HD2	2.47	0.40
1:A:300:MET:O	1:A:304:ARG:HG3	2.22	0.40
1:A:135:LEU:HD11	1:A:155:LEU:HD22	2.02	0.40
1:A:192:ALA:O	1:A:193:HIS:C	2.64	0.40
1:A:295:TYR:O	1:A:297:ASN:N	2.52	0.40

All (2) 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)
3:A:413:HOH:O	3:A:413:HOH:O[3_655]	2.08	0.12
1:A:70:TYR:OH	2:A:411:IK2:O1P[3_655]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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	399/401 (100%)	366 (92%)	27 (7%)	6 (2%)	8 16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	SER
1	A	202	GLN
1	A	263	TYR
1	A	296	SER
1	A	266	ARG
1	A	313	PRO

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	335/335 (100%)	291 (87%)	44 (13%)	4 8

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	18	LEU
1	A	37	VAL
1	A	46	LYS
1	A	50	LEU
1	A	55	LYS
1	A	68	LYS
1	A	79	PHE
1	A	80	THR
1	A	88	LEU
1	A	90	GLU
1	A	99	ARG
1	A	103	VAL
1	A	107	SER
1	A	129	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	138	PRO
1	A	168	LEU
1	A	179	LYS
1	A	184	SER
1	A	195	PRO
1	A	201	ARG
1	A	214	LYS
1	A	248	ILE
1	A	252	LEU
1	A	258	LYS
1	A	274	CYS
1	A	275	ARG
1	A	276	ASP
1	A	278	GLU
1	A	289	ILE
1	A	290	LEU
1	A	301	ASN
1	A	304	ARG
1	A	307	SER
1	A	314	GLU
1	A	321	VAL
1	A	343	LYS
1	A	351	GLN
1	A	366	LYS
1	A	373	LEU
1	A	375	LYS
1	A	383	LYS
1	A	409	THR
1	A	410	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	91	ASN
1	A	156	GLN
1	A	242	HIS
1	A	286	GLN
1	A	297	ASN
1	A	301	ASN
1	A	336	GLN
1	A	348	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	369	GLN
1	A	405	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	IK2	A	411	-	19,21,21	1.85	5 (26%)	24,29,29	4.24	14 (58%)

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	IK2	A	411	-	-	6/11/13/13	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	411	IK2	C5-C4	4.02	1.46	1.40
2	A	411	IK2	C3-C2	3.87	1.45	1.41
2	A	411	IK2	P-O3P	-2.74	1.44	1.54
2	A	411	IK2	O1'-C2'	2.52	1.30	1.22
2	A	411	IK2	C3-C4	-2.45	1.36	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	411	IK2	C4A-C4-C3	9.57	132.70	119.98
2	A	411	IK2	O3-C3-C2	-8.42	100.14	117.58
2	A	411	IK2	C4A-C4-C5	-7.93	111.11	119.75
2	A	411	IK2	O3-C3-C4	6.60	137.33	118.18
2	A	411	IK2	O4P-C5A-C5	5.03	118.79	109.36
2	A	411	IK2	C3-C2-N1	-4.89	114.80	120.96
2	A	411	IK2	C5A-C5-C4	-4.08	114.07	122.67
2	A	411	IK2	O2'-C2'-O1'	-4.06	112.90	123.33
2	A	411	IK2	C6-C5-C4	3.99	121.08	118.06
2	A	411	IK2	C6-N1-C2	3.91	126.29	119.20
2	A	411	IK2	C5A-C5-C6	3.37	124.85	119.36
2	A	411	IK2	C5-C6-N1	-2.91	119.10	123.83
2	A	411	IK2	C2A-C2-N1	2.83	122.97	117.64
2	A	411	IK2	C3-C4-C5	-2.81	116.18	118.73

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	411	IK2	C3-C4-C4A-N4A
2	A	411	IK2	C5A-O4P-P-O2P
2	A	411	IK2	C5A-O4P-P-O3P
2	A	411	IK2	C5-C4-C4A-N4A
2	A	411	IK2	C5A-O4P-P-O1P
2	A	411	IK2	OX-C1'-C2'-O2'

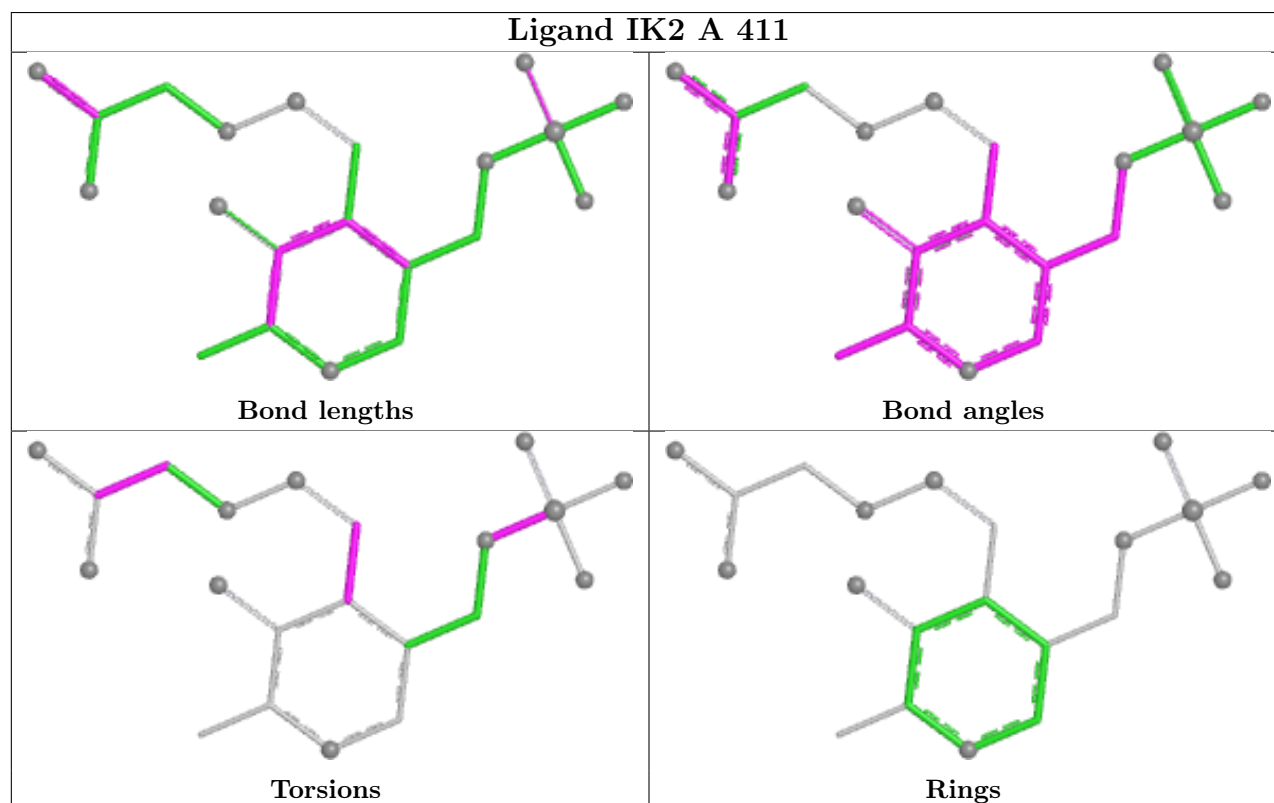
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	411	IK2	3	1

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.