



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 08:22 AM EDT

PDB ID : 1YBQ  
Title : Crystal structure of Escherichia coli isoaspartyl dipeptidase mutant D285N complexed with beta-aspartylhistidine  
Authors : Marti-Arbona, R.; Fresquet, V.; Thoden, J.B.; Davis, M.L.; Holden, H.M.; Raushel, F.M.  
Deposited on : 2004-12-21  
Resolution : 2.00 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](mailto: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 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) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

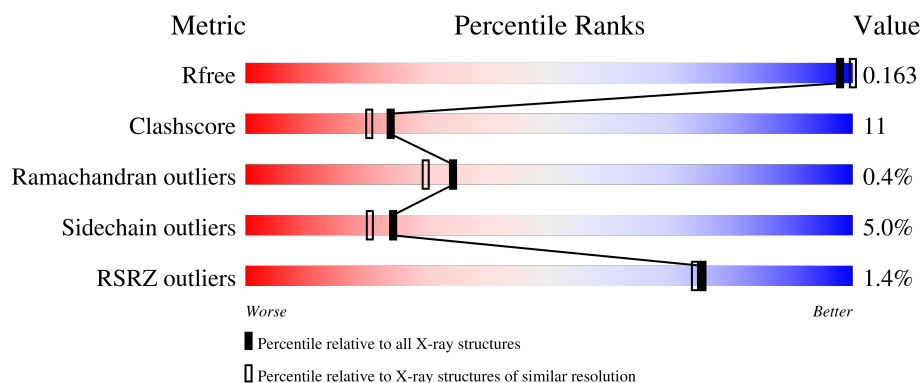
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	<div> <div>%</div> <div> <div></div> <div>65%</div> <div>32%</div> <div>.</div> </div> </div>
2	B	390	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>26%</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6054 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 Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	1	0
			2884	1816	496	560	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	285	ASN	ASP	engineered mutation	UNP P39377

- Molecule 2 is a protein called Isoaspartyl dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	389	Total	C	N	O	S	0	1	0
			2887	1817	496	562	12			

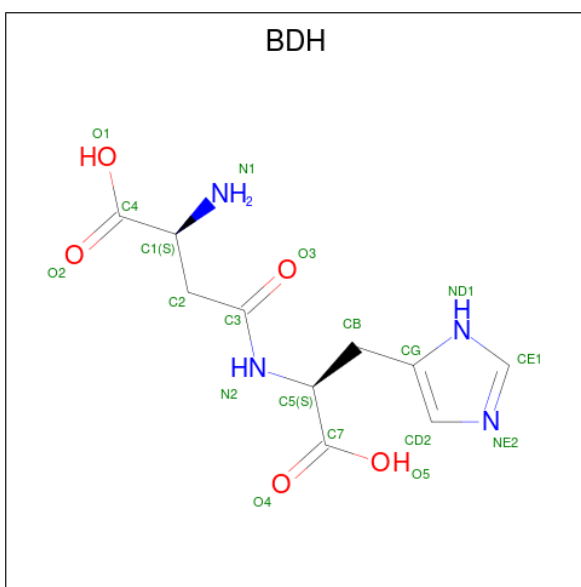
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	285	ASN	ASP	engineered mutation	UNP P39377

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is L-BETA-ASPARTYLHISTIDINE (three-letter code: BDH) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	10	4	5		
4	B	1	Total	C	N	O	0	0
			19	10	4	5		

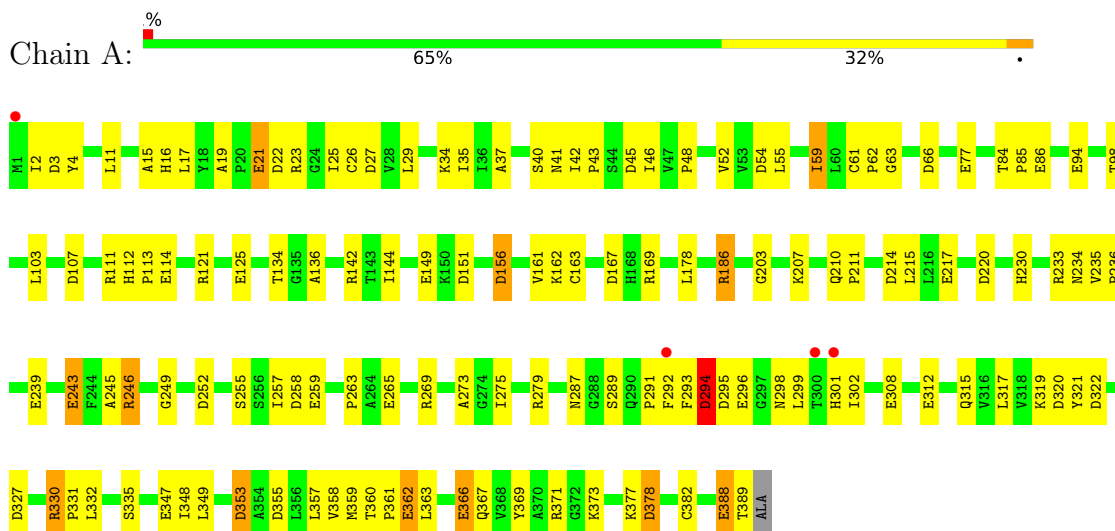
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	126	Total	O	0	0
			126	126		

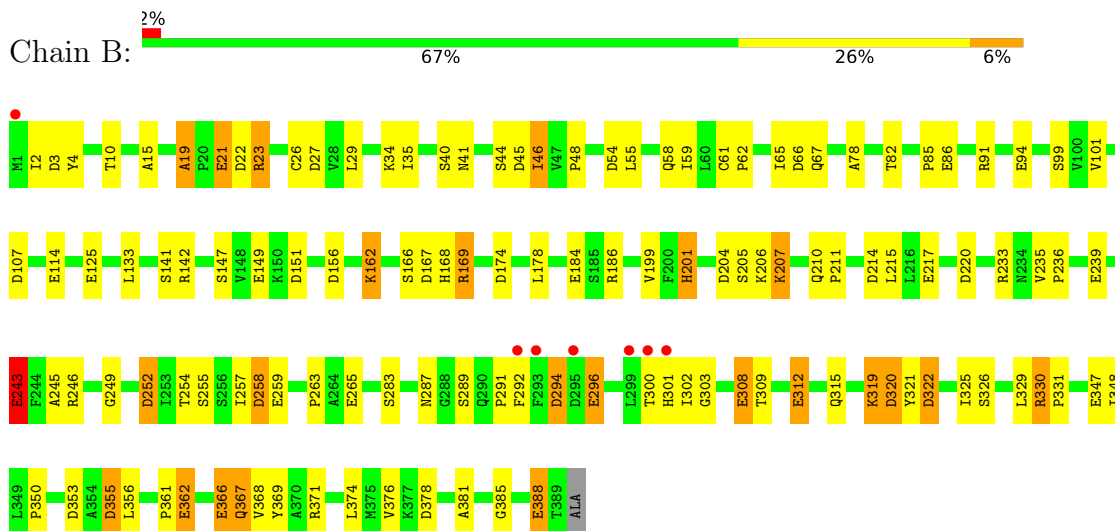
### 3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

- Molecule 1: Isoaspartyl dipeptidase



- Molecule 2: Isoaspartyl dipeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.30Å 119.30Å 138.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 38.22 – 1.92	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 82.8 (38.22-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 1.92Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.181 , 0.243 0.161 , 0.163	Depositor DCC
$R_{free}$ test set	6571 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.0	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 90.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6054	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, BDH, ZN

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	0.95	19/2938 (0.6%)	1.44	51/3998 (1.3%)
2	B	0.96	20/2928 (0.7%)	1.43	47/3984 (1.2%)
All	All	0.95	39/5866 (0.7%)	1.44	98/7982 (1.2%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	GLU	CD-OE2	9.08	1.35	1.25
2	B	217	GLU	CD-OE2	8.82	1.35	1.25
2	B	362	GLU	CD-OE2	7.82	1.34	1.25
2	B	312	GLU	CD-OE2	7.75	1.34	1.25
1	A	296	GLU	CD-OE2	7.69	1.34	1.25
1	A	217	GLU	CD-OE2	7.62	1.34	1.25
1	A	243	GLU	CD-OE2	7.04	1.33	1.25
2	B	296	GLU	CD-OE2	7.03	1.33	1.25
1	A	308	GLU	CD-OE2	6.92	1.33	1.25
1	A	312	GLU	CD-OE2	6.72	1.33	1.25
1	A	366	GLU	CD-OE2	6.70	1.33	1.25
1	A	21	GLU	CD-OE2	6.68	1.33	1.25
2	B	265	GLU	CD-OE2	6.65	1.32	1.25
1	A	239	GLU	CD-OE2	6.58	1.32	1.25
1	A	259	GLU	CD-OE2	6.48	1.32	1.25
2	B	388	GLU	CD-OE2	6.45	1.32	1.25
2	B	366	GLU	CD-OE2	6.38	1.32	1.25
2	B	149	GLU	CD-OE2	6.36	1.32	1.25
2	B	259	GLU	CD-OE2	6.17	1.32	1.25
1	A	265	GLU	CD-OE2	6.02	1.32	1.25
2	B	125	GLU	CD-OE2	5.80	1.32	1.25
2	B	243	GLU	CD-OE2	5.68	1.31	1.25
2	B	347	GLU	CD-OE2	5.58	1.31	1.25
1	A	86	GLU	CD-OE2	5.56	1.31	1.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	308	GLU	CD-OE2	5.53	1.31	1.25
2	B	94	GLU	CD-OE2	5.41	1.31	1.25
2	B	86	GLU	CD-OE1	-5.40	1.19	1.25
1	A	114	GLU	CD-OE2	5.36	1.31	1.25
2	B	184	GLU	CD-OE2	5.33	1.31	1.25
1	A	77	GLU	CD-OE2	5.32	1.31	1.25
1	A	94	GLU	CD-OE2	5.27	1.31	1.25
2	B	114	GLU	CD-OE2	5.23	1.31	1.25
1	A	125	GLU	CD-OE2	5.19	1.31	1.25
2	B	86	GLU	CD-OE2	5.18	1.31	1.25
2	B	21	GLU	CD-OE2	5.18	1.31	1.25
1	A	388	GLU	CD-OE2	5.09	1.31	1.25
1	A	149	GLU	CD-OE2	5.06	1.31	1.25
1	A	347	GLU	CD-OE2	5.05	1.31	1.25
2	B	239	GLU	CD-OE2	5.05	1.31	1.25

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	355	ASP	CB-CG-OD2	-10.15	109.16	118.30
2	B	169	ARG	NE-CZ-NH2	-10.13	115.24	120.30
2	B	66	ASP	CB-CG-OD2	-9.21	110.01	118.30
1	A	107	ASP	CB-CG-OD1	9.18	126.56	118.30
1	A	66	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	A	107	ASP	CB-CG-OD2	-9.05	110.16	118.30
2	B	23	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	A	322	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	A	169	ARG	NE-CZ-NH2	-8.55	116.03	120.30
2	B	252	ASP	CB-CG-OD1	8.31	125.78	118.30
2	B	355	ASP	CB-CG-OD1	8.08	125.57	118.30
2	B	252	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	A	330	ARG	NE-CZ-NH1	7.95	124.27	120.30
2	B	66	ASP	CB-CG-OD1	7.94	125.44	118.30
1	A	142	ARG	NE-CZ-NH1	7.91	124.25	120.30
2	B	107	ASP	CB-CG-OD1	7.86	125.38	118.30
1	A	169	ARG	NE-CZ-NH1	7.85	124.22	120.30
2	B	27	ASP	CB-CG-OD2	-7.79	111.28	118.30
2	B	378	ASP	CB-CG-OD2	-7.77	111.31	118.30
2	B	54	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	A	151	ASP	CB-CG-OD1	7.38	124.94	118.30
2	B	142	ARG	NE-CZ-NH1	7.33	123.96	120.30
1	A	353	ASP	CB-CG-OD2	-7.24	111.78	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASP	CB-CG-OD1	7.22	124.80	118.30
2	B	91	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	A	322	ASP	CB-CG-OD1	7.15	124.73	118.30
2	B	142	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	A	54	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	252	ASP	CB-CG-OD1	7.02	124.62	118.30
1	A	156	ASP	CB-CG-OD2	-6.97	112.03	118.30
2	B	233	ARG	NE-CZ-NH1	6.93	123.76	120.30
2	B	322	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	220	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	355	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	22	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	151	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	295	ASP	CB-CG-OD2	-6.79	112.19	118.30
2	B	107	ASP	CB-CG-OD2	-6.79	112.19	118.30
2	B	156	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	330	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	186	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	294	ASP	CB-CG-OD2	-6.64	112.32	118.30
2	B	214	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	A	220	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	378	ASP	CB-CG-OD2	-6.63	112.34	118.30
2	B	353	ASP	CB-CG-OD2	-6.61	112.35	118.30
2	B	322	ASP	CB-CG-OD2	-6.57	112.39	118.30
2	B	54	ASP	CB-CG-OD1	6.50	124.14	118.30
1	A	66	ASP	CB-CG-OD1	6.42	124.07	118.30
2	B	220	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	371	ARG	NE-CZ-NH1	6.37	123.49	120.30
2	B	151	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	353	ASP	CB-CG-OD1	6.34	124.01	118.30
1	A	27	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	A	111	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	258	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	327	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	45	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	B	156	ASP	CB-CG-OD1	6.06	123.76	118.30
2	B	4	TYR	CB-CG-CD2	-6.03	117.38	121.00
1	A	45	ASP	CB-CG-OD1	6.00	123.70	118.30
2	B	258	ASP	CB-CG-OD2	-6.00	112.91	118.30
1	A	54	ASP	CB-CG-OD1	5.96	123.66	118.30
2	B	3	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	269	ARG	NE-CZ-NH1	5.94	123.27	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	214	ASP	CB-CG-OD2	-5.91	112.98	118.30
2	B	330	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	B	294	ASP	CB-CG-OD2	-5.89	113.00	118.30
2	B	3	ASP	CB-CG-OD1	5.80	123.52	118.30
2	B	204	ASP	CB-CG-OD2	-5.80	113.08	118.30
2	B	26	CYS	N-CA-CB	-5.78	100.19	110.60
1	A	214	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	378	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	371	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	B	151	ASP	CB-CG-OD1	5.62	123.35	118.30
2	B	378	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	252	ASP	CB-CG-OD2	-5.55	113.31	118.30
2	B	174	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	294	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	279	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	167	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	B	22	ASP	CB-CG-OD2	-5.49	113.36	118.30
2	B	330	ARG	NE-CZ-NH1	5.45	123.02	120.30
2	B	174	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	320	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	3	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	246	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	327	ASP	CB-CG-OD1	5.31	123.08	118.30
2	B	353	ASP	CB-CG-OD1	5.30	123.07	118.30
2	B	320	ASP	CB-CG-OD2	-5.28	113.55	118.30
2	B	169	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	355	ASP	CB-CG-OD1	5.22	122.99	118.30
2	B	45	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	3	ASP	CB-CG-OD1	5.08	122.88	118.30
2	B	4	TYR	CB-CG-CD1	5.08	124.05	121.00
2	B	309	THR	CA-CB-CG2	-5.03	105.35	112.40
1	A	19	ALA	N-CA-C	5.01	124.53	111.00

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	2884	0	2911	67	0
2	B	2887	0	2908	65	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	19	0	12	0	0
4	B	19	0	12	0	0
5	A	115	0	0	1	0
5	B	126	0	0	0	1
All	All	6054	0	5843	129	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 11.

All (129) 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:254:THR:HB	2:B:257:ILE:HD12	1.38	1.05
2:B:243:GLU:HG3	2:B:246:ARG:NH1	1.90	0.87
2:B:254:THR:HB	2:B:257:ILE:CD1	2.04	0.86
2:B:243:GLU:HG3	2:B:246:ARG:HH12	1.40	0.84
2:B:235:VAL:HB	2:B:236:PRO:HD3	1.67	0.77
1:A:235:VAL:HB	1:A:236:PRO:HD3	1.69	0.75
1:A:294:ASP:HB3	1:A:298:ASN:H	1.51	0.75
1:A:330:ARG:HB2	1:A:331:PRO:HD3	1.69	0.74
2:B:348:ILE:HG12	2:B:356:LEU:CD2	2.17	0.73
2:B:330:ARG:HB2	2:B:331:PRO:HD3	1.71	0.72
1:A:16:HIS:HA	1:A:25:ILE:HD13	1.72	0.71
1:A:315:GLN:O	1:A:319:LYS:HB3	1.90	0.71
2:B:162:KCX:OQ2	2:B:201:HIS:HB2	1.92	0.69
1:A:294:ASP:CB	1:A:298:ASN:H	2.06	0.67
1:A:348:ILE:O	1:A:349:LEU:HD23	1.94	0.67
2:B:58:GLN:HA	2:B:58:GLN:HE21	1.59	0.67
1:A:257:ILE:O	1:A:263:PRO:HD3	1.95	0.66
2:B:166:SER:HB3	2:B:205:SER:HB3	1.76	0.66
2:B:292:PHE:HD1	2:B:301:HIS:HD1	1.42	0.66
2:B:308:GLU:O	2:B:312:GLU:HG3	1.96	0.66
1:A:294:ASP:HB2	1:A:298:ASN:O	1.98	0.64
1:A:294:ASP:OD2	1:A:298:ASN:HB2	1.97	0.64
2:B:133:LEU:HD11	2:B:199:VAL:HG21	1.80	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:ALA:HA	1:A:249:GLY:O	1.99	0.63
1:A:84:THR:HB	1:A:85:PRO:HD2	1.80	0.62
1:A:85:PRO:O	1:A:287:ASN:ND2	2.32	0.62
1:A:358:VAL:HG21	1:A:367:GLN:HE21	1.63	0.61
1:A:121:ARG:NH2	1:A:156:ASP:OD1	2.31	0.61
2:B:205:SER:OG	2:B:207:LYS:HG3	2.01	0.60
1:A:178:LEU:HB3	1:A:215:LEU:HD12	1.84	0.60
2:B:348:ILE:HG12	2:B:356:LEU:HD21	1.83	0.59
1:A:21:GLU:H	1:A:21:GLU:CD	2.06	0.59
2:B:85:PRO:O	2:B:287:ASN:ND2	2.35	0.58
1:A:42:ILE:HG23	1:A:43:PRO:HD2	1.85	0.58
2:B:61:CYS:HB2	2:B:62:PRO:CD	2.34	0.58
1:A:17:LEU:HD23	1:A:23:ARG:CB	2.33	0.58
1:A:289:SER:C	1:A:291:PRO:HD3	2.24	0.57
2:B:245:ALA:HA	2:B:249:GLY:O	2.04	0.57
1:A:17:LEU:HD23	1:A:23:ARG:HB2	1.84	0.57
1:A:360:THR:HB	1:A:361:PRO:HD2	1.87	0.57
2:B:19:ALA:CB	2:B:23:ARG:HH11	2.18	0.57
1:A:59:ILE:HD11	1:A:359:MET:CE	2.35	0.56
2:B:294:ASP:HB3	2:B:300:THR:HG21	1.86	0.56
1:A:42:ILE:HG12	2:B:2:ILE:HD13	1.87	0.55
2:B:319:LYS:HG2	2:B:320:ASP:N	2.22	0.54
1:A:230:HIS:O	1:A:233:ARG:HG2	2.08	0.54
2:B:19:ALA:HB3	2:B:23:ARG:NH1	2.21	0.54
2:B:215:LEU:C	2:B:215:LEU:HD23	2.27	0.54
1:A:15:ALA:HB2	1:A:55:LEU:HB2	1.90	0.52
1:A:61:CYS:HB2	1:A:62:PRO:CD	2.40	0.52
1:A:255:SER:HA	1:A:263:PRO:HG3	1.92	0.52
1:A:359:MET:CE	1:A:363:LEU:HD22	2.40	0.51
1:A:59:ILE:HD11	1:A:359:MET:HE3	1.90	0.51
1:A:34:LYS:NZ	1:A:353:ASP:OD1	2.34	0.51
2:B:355:ASP:C	2:B:356:LEU:HG	2.32	0.50
2:B:58:GLN:HA	2:B:58:GLN:NE2	2.24	0.50
2:B:294:ASP:HB3	2:B:300:THR:CG2	2.42	0.50
2:B:257:ILE:O	2:B:263:PRO:HD3	2.12	0.49
2:B:168:HIS:CD2	2:B:169:ARG:HG3	2.46	0.49
1:A:317:LEU:O	1:A:321:TYR:HB2	2.11	0.49
2:B:368:VAL:HB	2:B:376:VAL:HB	1.93	0.49
1:A:136:ALA:O	1:A:163:CYS:HA	2.12	0.49
1:A:377:LYS:O	1:A:378:ASP:HB2	2.12	0.49
2:B:315:GLN:O	2:B:319:LYS:HB3	2.11	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:CD1	1:A:292:PHE:N	2.81	0.49
2:B:78:ALA:HB3	2:B:82:THR:HG21	1.95	0.49
2:B:35:ILE:HD13	2:B:348:ILE:HG23	1.95	0.48
1:A:293:PHE:CZ	1:A:299:LEU:HD12	2.49	0.48
2:B:10:THR:O	2:B:29:LEU:HD12	2.12	0.48
1:A:167:ASP:HB2	1:A:203:GLY:HA3	1.95	0.48
2:B:289:SER:HB2	2:B:302:ILE:HD11	1.94	0.48
1:A:29:LEU:HB3	1:A:37:ALA:HB3	1.96	0.48
1:A:112:HIS:HD2	5:A:431:HOH:O	1.97	0.48
2:B:289:SER:C	2:B:291:PRO:HD3	2.34	0.48
1:A:162:LYS:HG3	1:A:163:CYS:N	2.29	0.47
1:A:359:MET:HE1	1:A:363:LEU:HD22	1.96	0.47
1:A:235:VAL:CB	1:A:236:PRO:HD3	2.41	0.47
2:B:19:ALA:CB	2:B:23:ARG:NH1	2.78	0.46
1:A:84:THR:HB	1:A:85:PRO:CD	2.46	0.45
1:A:302:ILE:O	1:A:302:ILE:HG23	2.16	0.45
2:B:321:TYR:O	2:B:322:ASP:HB3	2.16	0.45
1:A:234:ASN:OD1	1:A:236:PRO:HD2	2.16	0.45
2:B:58:GLN:HE21	2:B:58:GLN:CA	2.27	0.45
2:B:348:ILE:HG12	2:B:356:LEU:HD23	1.95	0.45
1:A:46:ILE:HG13	2:B:48:PRO:HG3	1.98	0.45
2:B:385:GLY:HA3	2:B:388:GLU:HG3	1.99	0.44
2:B:210:GLN:HB3	2:B:211:PRO:HD3	1.98	0.44
2:B:255:SER:HA	2:B:263:PRO:HG3	2.00	0.44
1:A:113:PRO:HB2	1:A:144:ILE:HG13	1.99	0.44
2:B:67:GLN:HA	2:B:101:VAL:HB	1.99	0.44
2:B:367:GLN:NE2	2:B:369:TYR:OH	2.51	0.44
1:A:63:GLY:HA2	1:A:357:LEU:HG	2.00	0.43
2:B:252:ASP:OD1	2:B:283:SER:OG	2.34	0.43
2:B:15:ALA:HB2	2:B:55:LEU:HB3	2.00	0.43
1:A:11:LEU:HD23	1:A:52:VAL:HG13	2.00	0.43
1:A:366:GLU:O	1:A:378:ASP:N	2.52	0.43
2:B:61:CYS:C	2:B:348:ILE:HD11	2.38	0.43
1:A:63:GLY:HA3	1:A:98:THR:OG1	2.18	0.43
2:B:61:CYS:HB2	2:B:62:PRO:HD2	2.00	0.43
2:B:178:LEU:HB3	2:B:215:LEU:HD12	1.99	0.43
1:A:61:CYS:HB2	1:A:62:PRO:HD2	2.01	0.43
1:A:273:ALA:HB3	1:A:275:ILE:HD12	2.00	0.43
2:B:235:VAL:CB	2:B:236:PRO:HD3	2.40	0.43
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.82	0.42
1:A:369:TYR:HA	1:A:373:LYS:O	2.19	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:VAL:HG22	2:B:381:ALA:HA	2.01	0.42
2:B:59:ILE:HD12	2:B:361:PRO:HA	2.01	0.42
1:A:178:LEU:HD23	1:A:178:LEU:HA	1.87	0.42
1:A:388:GLU:O	1:A:389:THR:HG23	2.20	0.42
2:B:35:ILE:HG22	2:B:350:PRO:HA	2.01	0.42
2:B:19:ALA:HB3	2:B:23:ARG:HH11	1.79	0.41
2:B:325:ILE:O	2:B:329:LEU:HG	2.20	0.41
1:A:134:THR:HG23	1:A:161:VAL:HG23	2.03	0.41
1:A:294:ASP:HB2	1:A:298:ASN:CA	2.50	0.41
1:A:215:LEU:C	1:A:215:LEU:HD23	2.41	0.41
1:A:2:ILE:CG2	1:A:4:TYR:CZ	3.03	0.41
1:A:35:ILE:HD13	1:A:348:ILE:HG23	2.03	0.41
1:A:331:PRO:HA	1:A:335:SER:HB2	2.03	0.41
1:A:358:VAL:HG21	1:A:367:GLN:NE2	2.31	0.41
1:A:235:VAL:CB	1:A:236:PRO:CD	2.98	0.41
1:A:210:GLN:N	1:A:211:PRO:CD	2.82	0.41
2:B:21:GLU:OE2	2:B:330:ARG:NH2	2.53	0.41
2:B:65:ILE:HG12	2:B:99:SER:HB2	2.03	0.41
2:B:289:SER:HA	2:B:303:GLY:O	2.20	0.40
2:B:374:LEU:HD11	2:B:376:VAL:O	2.22	0.40
1:A:48:PRO:HG3	2:B:46:ILE:HG13	2.03	0.40
2:B:21:GLU:H	2:B:21:GLU:CD	2.25	0.40
2:B:61:CYS:CB	2:B:62:PRO:CD	2.99	0.40
2:B:166:SER:CB	2:B:205:SER:HB3	2.49	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)
5:B:519:HOH:O	5:B:519:HOH:O[7_556]	1.95	0.25

## 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	388/390 (100%)	365 (94%)	21 (5%)	2 (0%)	29	23
2	B	387/390 (99%)	372 (96%)	14 (4%)	1 (0%)	41	37
All	All	775/780 (99%)	737 (95%)	35 (4%)	3 (0%)	34	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	A	41	ASN
2	B	19	ALA

### 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	314/313 (100%)	303 (96%)	11 (4%)	36	35
2	B	313/312 (100%)	293 (94%)	20 (6%)	17	13
All	All	627/625 (100%)	596 (95%)	31 (5%)	24	21

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	CYS
1	A	40	SER
1	A	59	ILE
1	A	103	LEU
1	A	186	ARG
1	A	207	LYS
1	A	243	GLU
1	A	246	ARG
1	A	301	HIS
1	A	362	GLU
1	A	382	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	34	LYS
2	B	40	SER
2	B	41	ASN
2	B	44	SER
2	B	46	ILE
2	B	141	SER
2	B	147	SER
2	B	186	ARG
2	B	201	HIS
2	B	206	LYS
2	B	207	LYS
2	B	243	GLU
2	B	258	ASP
2	B	296	GLU
2	B	319	LYS
2	B	326	SER
2	B	362	GLU
2	B	366	GLU
2	B	367	GLN
2	B	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	301	HIS
1	A	315	GLN
1	A	367	GLN
2	B	13	GLN
2	B	58	GLN
2	B	168	HIS
2	B	290	GLN
2	B	367	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



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

1 non-standard protein/DNA/RNA residue 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	KCX	B	162	2	7,11,12	0.66	0	4,12,14	4.76	1 (25%)

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	KCX	B	162	2	-	0/7/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	KCX	CE-NZ-CX	-9.43	106.98	122.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	162	KCX	1	0

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
4	BDH	A	393	3	9,19,19	3.81	3 (33%)	9,25,25	1.98	4 (44%)
4	BDH	B	393	3	9,19,19	3.77	3 (33%)	9,25,25	1.41	1 (11%)

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
4	BDH	A	393	3	-	5/12/20/20	0/1/1/1
4	BDH	B	393	3	-	4/12/20/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	393	BDH	C5-N2	-9.49	1.34	1.46
4	A	393	BDH	C5-N2	-9.05	1.34	1.46
4	A	393	BDH	C1-N1	-5.93	1.33	1.47
4	B	393	BDH	C1-N1	-5.37	1.35	1.47
4	A	393	BDH	CB-C5	3.28	1.58	1.53
4	B	393	BDH	CB-C5	2.36	1.57	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	393	BDH	CB-C5-N2	3.31	115.03	109.01
4	A	393	BDH	C2-C1-C4	-2.78	106.19	110.69
4	B	393	BDH	O3-C3-C2	-2.63	117.65	121.50
4	A	393	BDH	O3-C3-C2	-2.50	117.83	121.50
4	A	393	BDH	C1-C2-C3	-2.30	106.09	112.73

There are no chirality outliers.

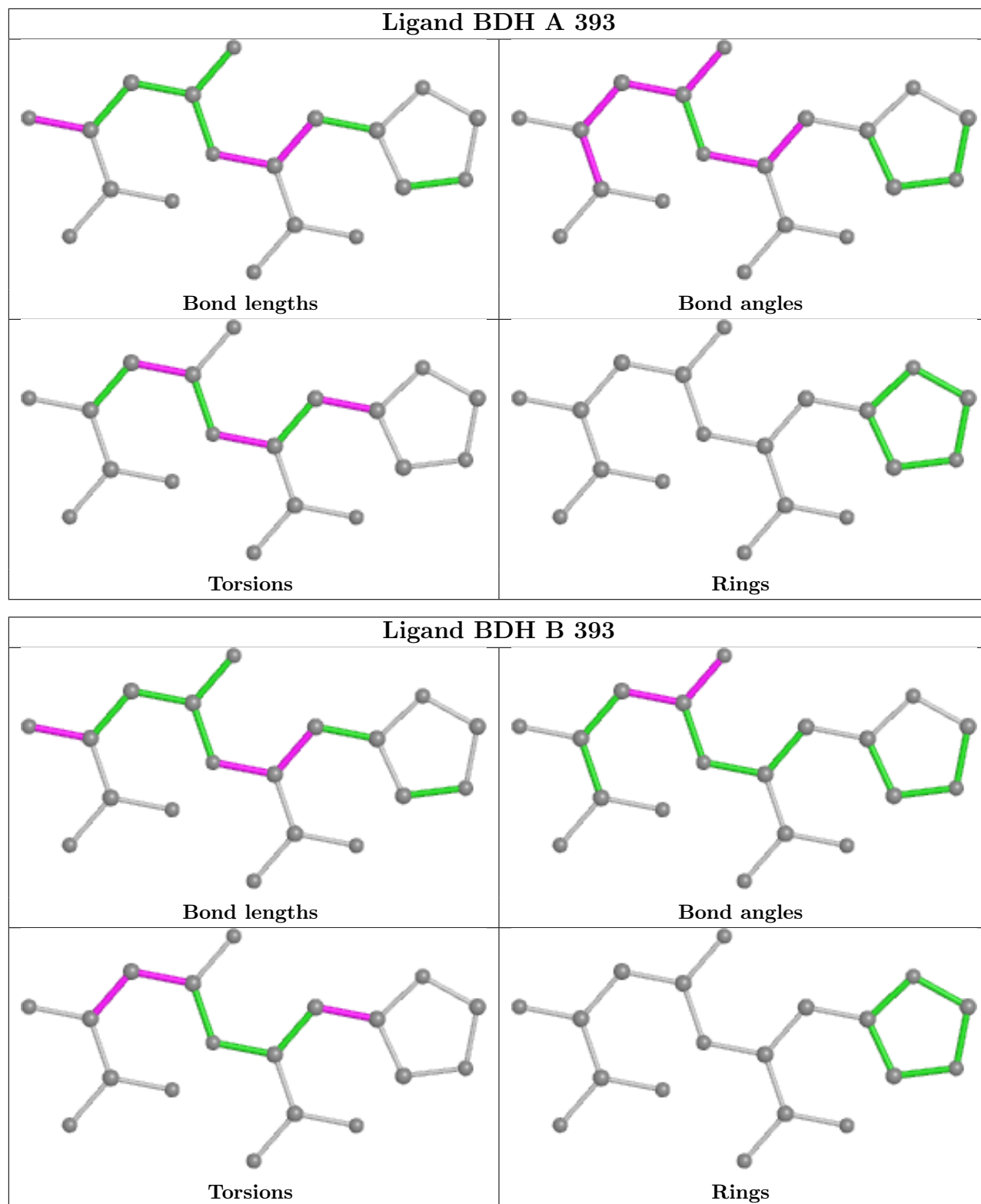
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	393	BDH	C5-CB-CG-ND1
4	B	393	BDH	C1-C2-C3-O3
4	B	393	BDH	C1-C2-C3-N2
4	A	393	BDH	CB-C5-N2-C3
4	B	393	BDH	C5-CB-CG-ND1
4	B	393	BDH	N1-C1-C2-C3
4	A	393	BDH	C7-C5-N2-C3
4	A	393	BDH	C1-C2-C3-O3
4	A	393	BDH	C5-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	389/390 (99%)	-0.66	4 (1%) 82 81	17, 30, 64, 100	0
2	B	388/390 (99%)	-0.56	7 (1%) 68 66	16, 30, 64, 100	0
All	All	777/780 (99%)	-0.61	11 (1%) 75 74	16, 30, 65, 100	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	301	HIS	5.7
2	B	292	PHE	5.0
2	B	299	LEU	3.2
2	B	295	ASP	3.2
2	B	293	PHE	3.0
2	B	1	MET	2.9
1	A	292	PHE	2.8
1	A	1	MET	2.6
1	A	300	THR	2.1
2	B	300	THR	2.0
1	A	301	HIS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	KCX	B	162	12/13	0.93	0.19	16,25,38,41	3

## 6.3 Carbohydrates [i](#)

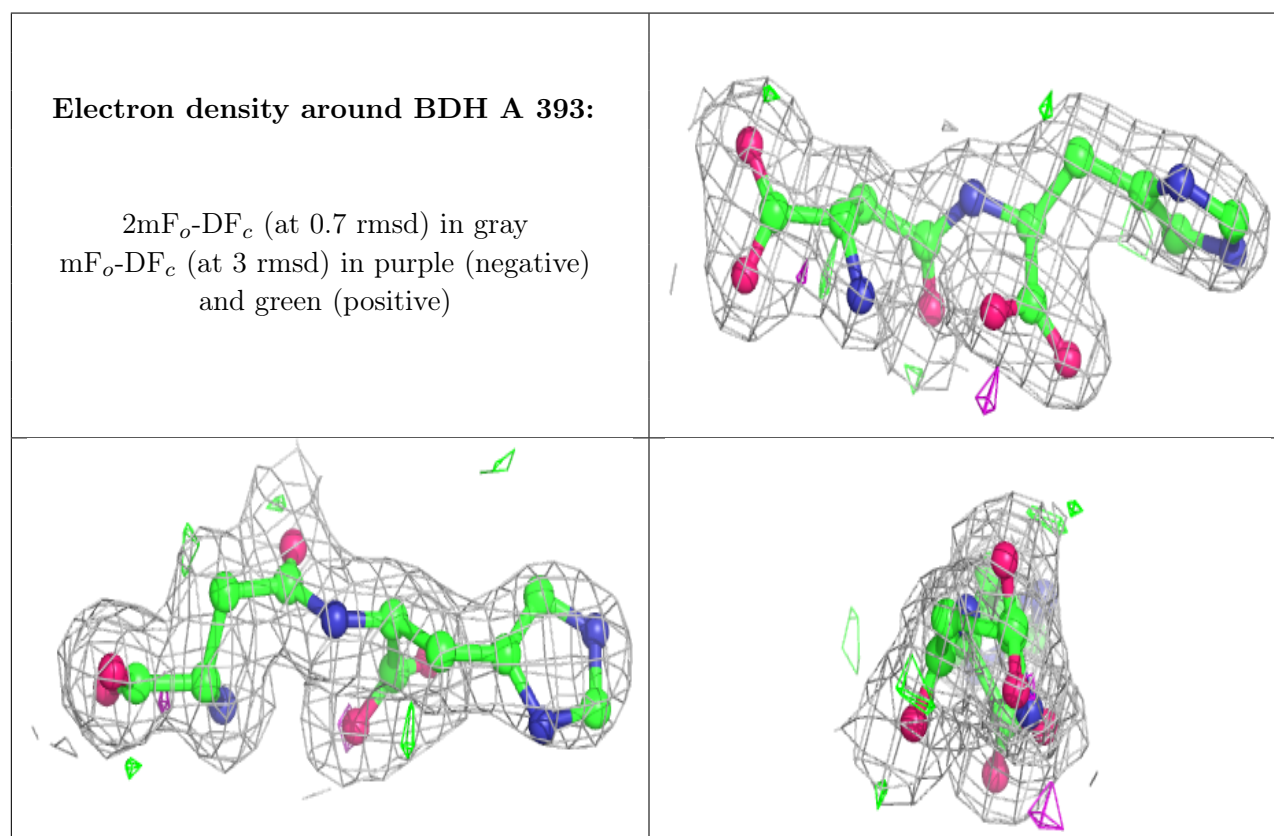
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

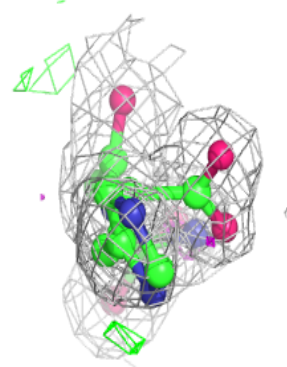
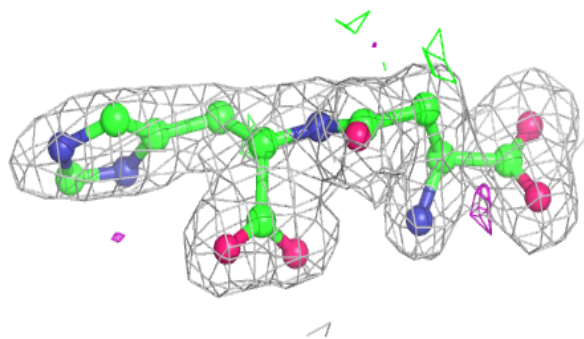
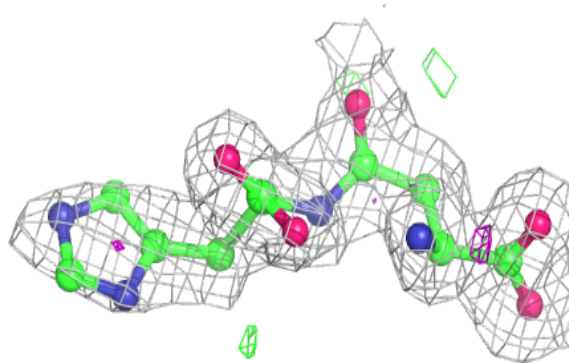
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	A	392	1/1	0.88	0.17	32,32,32,32	1
3	ZN	B	392	1/1	0.88	0.26	29,29,29,29	1
4	BDH	A	393	19/19	0.95	0.10	21,43,90,90	0
4	BDH	B	393	19/19	0.95	0.12	21,49,90,90	0
3	ZN	B	391	1/1	0.98	0.22	21,21,21,21	1
3	ZN	A	391	1/1	0.99	0.11	28,28,28,28	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around BDH B 393:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.