Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 09:49 PM EDT

PDB ID	:	1NAW
Title	:	ENOLPYRUVYL TRANSFERASE
Authors	:	Schoenbrunn, E.; Sack, S.; Eschenburg, S.; Perrakis, A.; Krekel, F.; Amrhein, N.; Mandelkow, E.
Deposited on	:	1996-07-23
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

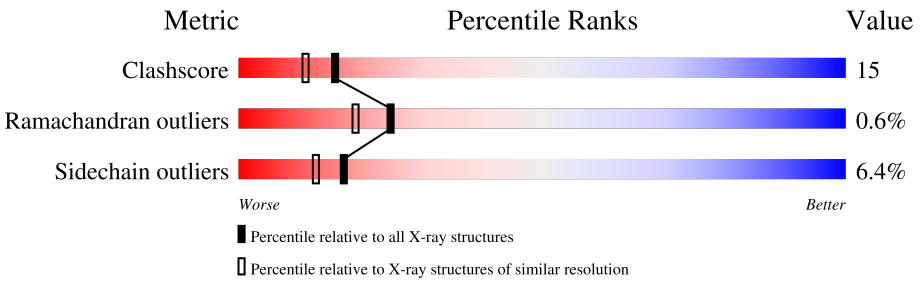
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	419	57% 36% 6% •
1	B	419	66% 25% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HAI	A	480	-	-	X	-

2 Entry composition (i)

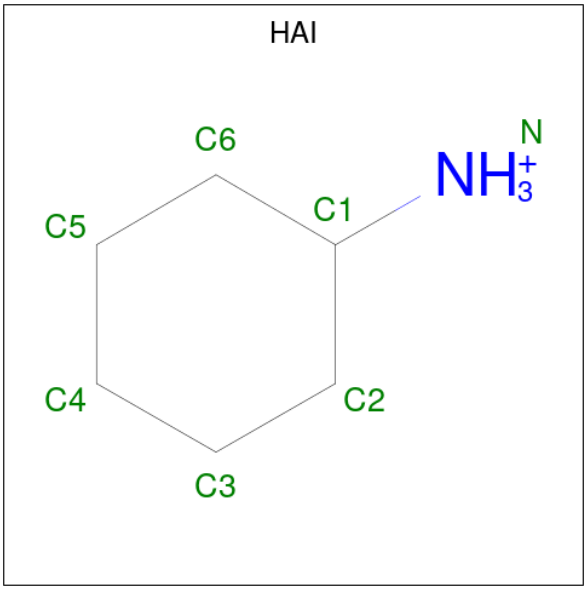
There are 3 unique types of molecules in this entry. The entry contains 6776 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-N-ACETYLGLUCOSAMINE 1-CARBOXYVINYL-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3142	1976	555	597	14	0	0	0
1	B	419	3142	1976	555	597	14	0	0	0

- Molecule 2 is CYCLOHEXYLAMMONIUM ION (three-letter code: HAI) (formula: $C_6H_{14}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	N		
2	A	1	7	6	1	0	0
2	A	1	7	6	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	242	242	242	0	0
			Total	O		
3	B	236	236	236	0	0

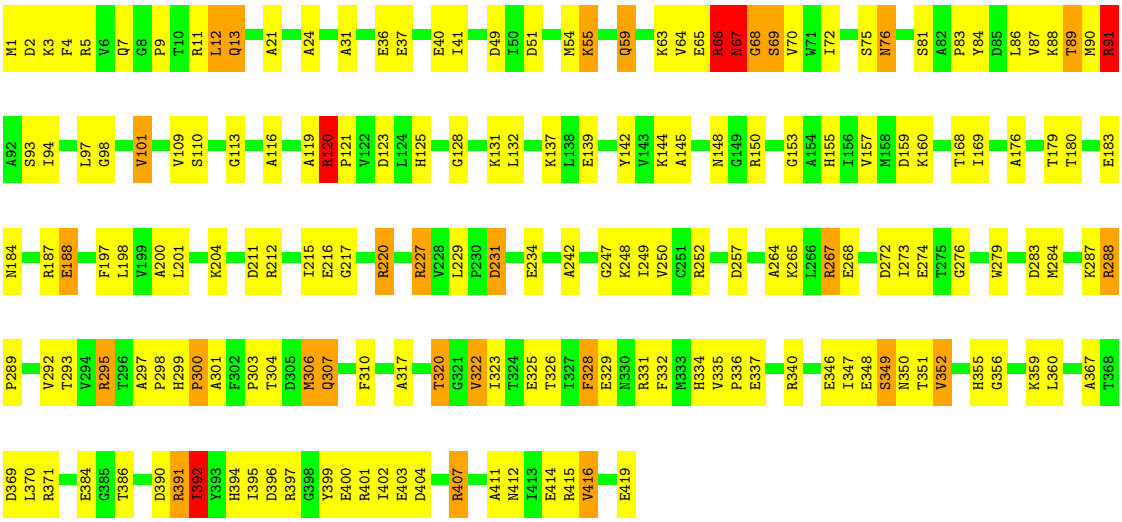
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

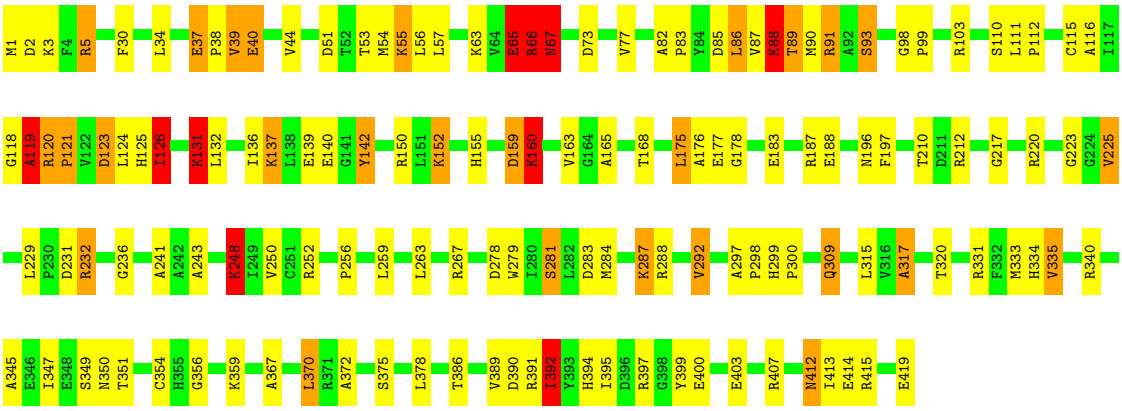
• Molecule 1: UDP-N-ACETYLGLUCOSAMINE 1-CARBOXYVINYL-TRANSFERASE

Chain A:



• Molecule 1: UDP-N-ACETYLGLUCOSAMINE 1-CARBOXYVINYL-TRANSFERASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.90Å 155.90Å 83.85Å 90.00° 91.65° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	99.9 (10.00-2.00)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.197 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6776	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HAI

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	0.78	0/3187	2.28	127/4319 (2.9%)
1	B	0.81	0/3187	2.27	118/4319 (2.7%)
All	All	0.80	0/6374	2.28	245/8638 (2.8%)

There are no bond length outliers.

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	212	ARG	NE-CZ-NH1	25.33	132.97	120.30
1	A	150	ARG	CD-NE-CZ	23.67	156.74	123.60
1	A	391	ARG	NE-CZ-NH1	21.84	131.22	120.30
1	B	187	ARG	NE-CZ-NH2	-20.92	109.84	120.30
1	A	220	ARG	CD-NE-CZ	20.27	151.97	123.60
1	B	123	ASP	CB-CG-OD1	20.25	136.52	118.30
1	B	391	ARG	NE-CZ-NH2	-20.02	110.29	120.30
1	A	391	ARG	NE-CZ-NH2	-19.74	110.43	120.30
1	A	267	ARG	NE-CZ-NH2	-18.56	111.02	120.30
1	B	331	ARG	NE-CZ-NH2	18.11	129.35	120.30
1	A	211	ASP	CB-CG-OD1	16.95	133.55	118.30
1	A	331	ARG	NE-CZ-NH1	16.77	128.68	120.30
1	B	187	ARG	NE-CZ-NH1	16.65	128.62	120.30
1	A	150	ARG	NE-CZ-NH1	16.61	128.60	120.30
1	B	91	ARG	CD-NE-CZ	16.45	146.63	123.60
1	A	227	ARG	NE-CZ-NH1	-16.22	112.19	120.30
1	B	212	ARG	NE-CZ-NH2	-15.34	112.63	120.30
1	B	340	ARG	CD-NE-CZ	15.00	144.59	123.60
1	B	220	ARG	NE-CZ-NH2	-14.89	112.86	120.30
1	B	340	ARG	NE-CZ-NH1	13.51	127.06	120.30
1	A	252	ARG	NE-CZ-NH2	-13.27	113.66	120.30
1	A	371	ARG	NE-CZ-NH2	-13.02	113.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	391	ARG	CD-NE-CZ	12.93	141.70	123.60
1	B	5	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	A	407	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	B	66	ARG	NE-CZ-NH2	-12.57	114.02	120.30
1	B	91	ARG	NE-CZ-NH1	12.07	126.33	120.30
1	A	331	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	A	267	ARG	NH1-CZ-NH2	11.51	132.06	119.40
1	A	66	ARG	NE-CZ-NH2	-11.09	114.75	120.30
1	B	91	ARG	NE-CZ-NH2	-11.07	114.76	120.30
1	B	397	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	A	283	ASP	CB-CG-OD1	10.96	128.16	118.30
1	A	283	ASP	CB-CG-OD2	-10.81	108.57	118.30
1	B	232	ARG	CD-NE-CZ	10.71	138.59	123.60
1	A	211	ASP	CB-CG-OD2	-10.69	108.68	118.30
1	B	123	ASP	CB-CA-C	10.69	131.78	110.40
1	A	295	ARG	NE-CZ-NH1	-10.35	115.13	120.30
1	A	288	ARG	NE-CZ-NH2	10.14	125.37	120.30
1	B	331	ARG	CD-NE-CZ	10.12	137.76	123.60
1	A	272	ASP	CB-CG-OD1	9.91	127.22	118.30
1	B	91	ARG	CA-CB-CG	9.91	135.20	113.40
1	B	66	ARG	C-N-CA	9.84	146.29	121.70
1	A	369	ASP	CB-CG-OD1	9.83	127.14	118.30
1	A	123	ASP	CB-CG-OD1	9.75	127.08	118.30
1	B	391	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	120	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	257	ASP	CB-CG-OD1	9.54	126.88	118.30
1	A	288	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	B	67	ASN	CA-CB-CG	-9.40	92.71	113.40
1	A	212	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	A	401	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	A	220	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	A	415	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	B	232	ARG	NE-CZ-NH2	-9.15	115.73	120.30
1	B	5	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	B	340	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	A	150	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	B	248	LYS	CA-CB-CG	8.94	133.06	113.40
1	A	397	ARG	CD-NE-CZ	-8.91	111.12	123.60
1	B	252	ARG	NE-CZ-NH1	8.85	124.73	120.30
1	B	66	ARG	NH1-CZ-NH2	8.74	129.01	119.40
1	B	212	ARG	CD-NE-CZ	8.73	135.82	123.60
1	A	11	ARG	NE-CZ-NH1	-8.70	115.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	283	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	A	407	ARG	CD-NE-CZ	8.45	135.43	123.60
1	A	340	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	A	84	TYR	CB-CG-CD2	-8.41	115.95	121.00
1	B	414	GLU	CB-CG-CD	8.40	136.89	114.20
1	A	67	ASN	CA-C-N	8.37	132.94	116.20
1	A	68	GLY	N-CA-C	-8.37	92.19	113.10
1	A	220	ARG	CG-CD-NE	8.36	129.35	111.80
1	A	337	GLU	OE1-CD-OE2	-8.33	113.30	123.30
1	B	412	ASN	CB-CG-OD1	-8.30	105.01	121.60
1	A	414	GLU	OE1-CD-OE2	8.19	133.13	123.30
1	B	159	ASP	CB-CG-OD2	8.18	125.66	118.30
1	B	231	ASP	CB-CG-OD2	8.18	125.66	118.30
1	A	407	ARG	NH1-CZ-NH2	-8.10	110.49	119.40
1	A	67	ASN	CA-CB-CG	-8.09	95.60	113.40
1	B	351	THR	CA-CB-CG2	8.01	123.61	112.40
1	B	159	ASP	CB-CG-OD1	7.97	125.47	118.30
1	A	2	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	252	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	B	397	ARG	NH1-CZ-NH2	7.84	128.02	119.40
1	B	120	ARG	N-CA-CB	7.77	124.59	110.60
1	B	292	VAL	N-CA-CB	-7.76	94.44	111.50
1	A	187	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	A	88	LYS	C-N-CA	7.74	141.05	121.70
1	A	93	SER	O-C-N	-7.70	110.38	122.70
1	A	13	GLN	N-CA-CB	-7.64	96.84	110.60
1	B	400	GLU	OE1-CD-OE2	-7.61	114.17	123.30
1	B	159	ASP	OD1-CG-OD2	-7.60	108.86	123.30
1	A	65	GLU	CA-CB-CG	7.54	129.99	113.40
1	B	93	SER	O-C-N	-7.42	110.82	122.70
1	A	242	ALA	N-CA-CB	7.37	120.41	110.10
1	B	331	ARG	CG-CD-NE	7.36	127.24	111.80
1	B	123	ASP	OD1-CG-OD2	-7.33	109.38	123.30
1	A	220	ARG	NH1-CZ-NH2	-7.30	111.37	119.40
1	A	400	GLU	OE1-CD-OE2	-7.29	114.56	123.30
1	B	414	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	A	396	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	B	67	ASN	CA-C-N	7.15	130.49	116.20
1	B	283	ASP	CB-CG-OD1	7.14	124.73	118.30
1	B	267	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	331	ARG	NH1-CZ-NH2	-7.11	111.58	119.40
1	B	232	ARG	NE-CZ-NH1	7.09	123.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	ASN	N-CA-C	7.09	130.14	111.00
1	A	12	LEU	CA-C-O	7.04	134.89	120.10
1	A	231	ASP	CB-CG-OD2	7.03	124.62	118.30
1	A	188	GLU	OE1-CD-OE2	-7.02	114.88	123.30
1	B	115	CYS	CA-CB-SG	7.00	126.60	114.00
1	B	412	ASN	CB-CG-ND2	7.00	133.49	116.70
1	A	252	ARG	NH1-CZ-NH2	6.95	127.04	119.40
1	A	300	PRO	N-CA-C	6.91	130.05	112.10
1	A	220	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	267	ARG	CD-NE-CZ	-6.86	114.00	123.60
1	A	49	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	A	267	ARG	NE-CZ-NH1	-6.77	116.91	120.30
1	A	89	THR	CB-CA-C	-6.74	93.42	111.60
1	B	163	VAL	CA-CB-CG2	6.72	120.97	110.90
1	B	66	ARG	NE-CZ-NH1	-6.69	116.96	120.30
1	B	103	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	89	THR	N-CA-CB	-6.61	97.74	110.30
1	B	77	VAL	CA-CB-CG2	-6.60	100.99	110.90
1	B	91	ARG	CB-CG-CD	6.59	128.72	111.60
1	A	367	ALA	N-CA-CB	6.58	119.31	110.10
1	A	415	ARG	CD-NE-CZ	6.55	132.77	123.60
1	B	40	GLU	OE1-CD-OE2	6.52	131.12	123.30
1	B	392	ILE	CA-CB-CG2	6.51	123.93	110.90
1	B	287	LYS	CD-CE-NZ	6.49	126.61	111.70
1	A	69	SER	CB-CA-C	-6.44	97.87	110.10
1	A	37	GLU	OE1-CD-OE2	-6.43	115.58	123.30
1	A	66	ARG	CB-CA-C	-6.42	97.55	110.40
1	A	399	TYR	CB-CG-CD2	-6.41	117.16	121.00
1	A	397	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	59	GLN	CB-CG-CD	6.38	128.19	111.60
1	B	248	LYS	CB-CG-CD	6.37	128.17	111.60
1	A	55	LYS	CG-CD-CE	6.35	130.94	111.90
1	B	66	ARG	O-C-N	-6.32	112.58	122.70
1	B	412	ASN	N-CA-CB	6.31	121.96	110.60
1	A	187	ARG	NH1-CZ-NH2	6.30	126.33	119.40
1	A	400	GLU	CA-CB-CG	6.29	127.24	113.40
1	A	91	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	24	ALA	N-CA-CB	6.27	118.88	110.10
1	A	54	MET	CG-SD-CE	6.26	110.22	100.20
1	B	120	ARG	CA-CB-CG	6.26	127.17	113.40
1	B	225	VAL	CG1-CB-CG2	-6.26	100.89	110.90
1	B	350	ASN	OD1-CG-ND2	-6.25	107.53	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	397	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	350	ASN	O-C-N	-6.25	112.71	122.70
1	B	160	LYS	CA-CB-CG	6.20	127.05	113.40
1	B	187	ARG	CG-CD-NE	6.20	124.83	111.80
1	B	197	PHE	CB-CG-CD1	-6.19	116.47	120.80
1	A	93	SER	CB-CA-C	6.15	121.79	110.10
1	B	91	ARG	CG-CD-NE	6.15	124.72	111.80
1	B	256	PRO	O-C-N	-6.13	112.89	122.70
1	A	187	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	90	MET	N-CA-CB	-6.10	99.61	110.60
1	A	67	ASN	O-C-N	-6.08	112.87	123.20
1	A	68	GLY	CA-C-O	6.06	131.51	120.60
1	A	352	VAL	CB-CA-C	-6.06	99.89	111.40
1	A	68	GLY	CA-C-N	-6.04	103.91	117.20
1	B	51	ASP	CB-CG-OD1	6.03	123.73	118.30
1	A	369	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	274	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	B	142	TYR	CB-CG-CD1	5.94	124.57	121.00
1	B	39	VAL	CA-CB-CG1	5.93	119.80	110.90
1	B	66	ARG	CG-CD-NE	-5.93	99.35	111.80
1	B	65	GLU	CG-CD-OE1	5.90	130.10	118.30
1	B	123	ASP	N-CA-CB	-5.89	100.00	110.60
1	B	88	LYS	C-N-CA	5.88	136.41	121.70
1	B	212	ARG	CB-CG-CD	-5.88	96.33	111.60
1	B	55	LYS	CA-CB-CG	5.87	126.31	113.40
1	B	93	SER	CB-CA-C	5.86	121.22	110.10
1	B	132	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	B	196	ASN	CB-CG-OD1	5.83	133.26	121.60
1	A	252	ARG	CG-CD-NE	-5.82	99.58	111.80
1	A	349	SER	N-CA-CB	-5.82	101.78	110.50
1	A	322	VAL	CG1-CB-CG2	5.76	120.12	110.90
1	B	317	ALA	CB-CA-C	-5.75	101.47	110.10
1	A	328	PHE	CB-CA-C	-5.75	98.91	110.40
1	B	82	ALA	N-CA-CB	5.74	118.14	110.10
1	A	132	LEU	CB-CG-CD1	-5.73	101.25	111.00
1	A	113	GLY	N-CA-C	5.73	127.42	113.10
1	A	119	ALA	CB-CA-C	5.73	118.69	110.10
1	B	391	ARG	CD-NE-CZ	5.72	131.61	123.60
1	A	419	GLU	CA-C-O	5.71	132.09	120.10
1	B	349	SER	CB-CA-C	5.71	120.94	110.10
1	A	392	ILE	CA-CB-CG2	5.70	122.30	110.90
1	B	287	LYS	CA-CB-CG	5.68	125.90	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	187	ARG	CD-NE-CZ	5.68	131.55	123.60
1	B	66	ARG	N-CA-CB	-5.67	100.40	110.60
1	B	39	VAL	CG1-CB-CG2	-5.66	101.84	110.90
1	A	90	MET	N-CA-CB	-5.63	100.46	110.60
1	A	201	LEU	CA-C-N	5.61	127.41	116.20
1	A	306	MET	CG-SD-CE	5.59	109.15	100.20
1	A	322	VAL	CB-CA-C	-5.59	100.78	111.40
1	A	415	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	A	411	ALA	N-CA-CB	5.53	117.84	110.10
1	A	84	TYR	CB-CG-CD1	5.50	124.30	121.00
1	A	404	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	335	VAL	N-CA-CB	5.43	123.46	111.50
1	B	67	ASN	CA-C-O	-5.43	108.71	120.10
1	A	292	VAL	CG1-CB-CG2	-5.42	102.22	110.90
1	B	399	TYR	CB-CG-CD2	5.42	124.25	121.00
1	A	257	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	351	THR	N-CA-CB	5.42	120.60	110.30
1	A	66	ARG	C-N-CA	5.41	135.23	121.70
1	B	119	ALA	N-CA-CB	5.40	117.65	110.10
1	A	227	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	B	131	LYS	CB-CG-CD	5.33	125.46	111.60
1	B	292	VAL	CB-CA-C	5.33	121.52	111.40
1	B	399	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	A	234	GLU	OE1-CD-OE2	-5.31	116.93	123.30
1	B	281	SER	N-CA-CB	5.30	118.45	110.50
1	B	367	ALA	N-CA-CB	5.30	117.52	110.10
1	A	320	THR	O-C-N	5.29	132.20	123.20
1	A	49	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	40	GLU	CG-CD-OE2	-5.29	107.72	118.30
1	A	184	ASN	CA-C-O	5.23	131.08	120.10
1	A	351	THR	CB-CA-C	-5.23	97.48	111.60
1	B	73	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	178	GLY	CA-C-O	5.22	130.00	120.60
1	B	288	ARG	CA-CB-CG	5.21	124.87	113.40
1	A	407	ARG	CG-CD-NE	5.21	122.73	111.80
1	A	40	GLU	CA-CB-CG	-5.20	101.96	113.40
1	A	212	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	416	VAL	CA-C-O	5.19	130.99	120.10
1	B	391	ARG	C-N-CA	5.17	134.62	121.70
1	B	188	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	A	337	GLU	CG-CD-OE1	5.14	128.57	118.30
1	A	399	TYR	CB-CG-CD1	5.13	124.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	37	GLU	OE1-CD-OE2	-5.13	117.14	123.30
1	B	142	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	B	44	VAL	CB-CA-C	5.10	121.09	111.40
1	B	241	ALA	O-C-N	-5.10	114.54	122.70
1	B	165	ALA	N-CA-CB	5.09	117.23	110.10
1	A	159	ASP	C-N-CA	5.08	134.40	121.70
1	B	236	GLY	O-C-N	-5.07	114.59	122.70
1	A	371	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	407	ARG	CA-CB-CG	5.05	124.52	113.40
1	A	66	ARG	CG-CD-NE	-5.03	101.25	111.80
1	A	81	SER	CB-CA-C	5.03	119.65	110.10
1	A	407	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	B	126	ILE	CG1-CB-CG2	-5.01	100.39	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3142	0	3220	100	0
1	B	3142	0	3219	84	0
2	A	14	0	27	7	0
3	A	242	0	0	17	2
3	B	236	0	0	12	2
All	All	6776	0	6466	186	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 15.

All (186) 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:287:LYS:HE3	3:A:571:HOH:O	1.50	1.09
1:A:287:LYS:CE	3:A:571:HOH:O	1.98	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LYS:HZ1	1:B:419:GLU:HG3	1.22	1.02
1:B:335:VAL:HG22	1:B:347:ILE:HD11	1.50	0.91
1:B:137:LYS:NZ	1:B:137:LYS:HB3	1.87	0.87
1:B:83:PRO:HD2	1:B:86:LEU:HD12	1.57	0.85
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.42	0.82
1:A:139:GLU:HB2	1:A:142:TYR:CE2	2.16	0.81
2:A:479:HAI:H41	2:A:480:HAI:H41	1.63	0.81
1:A:287:LYS:HE2	3:A:571:HOH:O	1.72	0.78
1:B:248:LYS:NZ	1:B:281:SER:HB2	1.98	0.78
1:B:392:ILE:HD12	1:B:395:ILE:HD12	1.67	0.76
1:B:120:ARG:HB3	1:B:121:PRO:HD2	1.68	0.76
1:B:121:PRO:O	3:B:645:HOH:O	2.03	0.76
1:A:91:ARG:HH12	1:A:121:PRO:HG2	1.51	0.75
1:A:101:VAL:HG11	1:A:145:ALA:HB3	1.69	0.74
1:B:3:LYS:NZ	1:B:419:GLU:HG3	2.01	0.74
1:A:116:ALA:O	1:A:120:ARG:HD2	1.87	0.74
1:A:284:MET:O	1:A:287:LYS:HE2	1.88	0.74
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.69	0.73
1:B:54:MET:SD	1:B:66:ARG:HG3	2.28	0.73
1:B:278:ASP:OD1	3:B:546:HOH:O	2.07	0.72
1:B:131:LYS:NZ	1:B:131:LYS:HB3	2.06	0.71
1:A:51:ASP:O	1:A:55:LYS:HD3	1.90	0.71
1:B:248:LYS:HZ1	1:B:281:SER:HB2	1.56	0.71
1:A:347:ILE:HD13	1:A:352:VAL:HG22	1.72	0.70
1:B:34:LEU:HD22	1:B:175:LEU:HD22	1.72	0.70
1:B:299:HIS:HD2	3:B:421:HOH:O	1.75	0.70
1:A:265:LYS:HE3	1:A:268:GLU:OE1	1.92	0.70
1:B:1:MET:N	1:B:419:GLU:HB2	2.07	0.69
1:B:98:GLY:HA3	3:B:570:HOH:O	1.91	0.69
1:B:309:GLN:HE21	1:B:309:GLN:H	1.43	0.66
1:B:139:GLU:HB2	1:B:142:TYR:CE1	2.31	0.65
1:A:299:HIS:HD2	3:A:494:HOH:O	1.78	0.65
1:A:346:GLU:OE1	1:A:355:HIS:HE1	1.81	0.64
1:B:155:HIS:HE1	1:B:183:GLU:OE2	1.81	0.64
1:B:37:GLU:HB3	1:B:38:PRO:HD2	1.78	0.63
1:A:287:LYS:NZ	3:A:705:HOH:O	2.31	0.63
1:A:394:HIS:HD2	3:A:578:HOH:O	1.82	0.63
1:A:334:HIS:H	1:A:334:HIS:CD2	2.17	0.62
1:A:89:THR:HG22	3:A:554:HOH:O	2.00	0.61
1:B:123:ASP:HB2	3:B:535:HOH:O	1.99	0.61
1:A:98:GLY:HA3	3:A:497:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ALA:O	1:B:217:GLY:HA3	2.00	0.61
1:A:307:GLN:HG2	1:A:323:ILE:HG21	1.81	0.61
1:B:120:ARG:HB3	1:B:121:PRO:CD	2.31	0.61
1:A:204:LYS:HD3	1:A:216:GLU:OE1	2.01	0.60
2:A:480:HAI:H31	1:B:279:TRP:CD1	2.37	0.60
1:B:394:HIS:HB2	3:B:554:HOH:O	2.02	0.59
1:B:137:LYS:HB3	1:B:137:LYS:HZ3	1.66	0.59
1:A:97:LEU:O	1:A:101:VAL:HG13	2.05	0.57
1:B:99:PRO:HD3	3:B:570:HOH:O	2.02	0.57
1:B:177:GLU:O	1:B:177:GLU:HG3	2.04	0.57
1:A:125:HIS:HD2	1:A:168:THR:OG1	1.88	0.57
1:B:3:LYS:HZ1	1:B:419:GLU:CG	2.08	0.56
1:A:347:ILE:CD1	1:A:352:VAL:HG22	2.36	0.56
1:A:250:VAL:HG11	2:A:480:HAI:H32	1.87	0.56
1:A:297:ALA:HB3	1:A:301:ALA:CB	2.36	0.55
1:B:2:ASP:OD2	1:B:415:ARG:HD3	2.05	0.55
1:A:265:LYS:HE2	1:A:293:THR:O	2.06	0.55
1:B:131:LYS:HB3	1:B:131:LYS:HZ3	1.71	0.55
1:B:89:THR:HG22	3:B:497:HOH:O	2.06	0.55
1:B:248:LYS:HZ2	1:B:281:SER:HB2	1.72	0.55
1:A:176:ALA:O	1:A:217:GLY:HA3	2.06	0.55
2:A:480:HAI:H52	1:B:250:VAL:HG11	1.89	0.55
1:B:118:GLY:O	1:B:119:ALA:C	2.45	0.54
1:A:299:HIS:CD2	3:A:494:HOH:O	2.58	0.54
1:A:329:GLU:HB3	3:A:665:HOH:O	2.08	0.54
1:B:66:ARG:NH2	1:B:67:ASN:O	2.23	0.54
1:A:317:ALA:O	1:A:356:GLY:HA3	2.07	0.54
1:B:124:LEU:HD11	1:B:160:LYS:HG2	1.88	0.54
1:A:155:HIS:HE1	1:A:183:GLU:OE2	1.90	0.54
1:B:243:ALA:HA	1:B:284:MET:CG	2.38	0.54
1:B:297:ALA:HB1	1:B:298:PRO:CD	2.38	0.53
1:A:59:GLN:HE21	1:A:86:LEU:HD11	1.73	0.53
1:A:297:ALA:HB1	1:A:298:PRO:HD2	1.91	0.52
1:A:188:GLU:OE1	1:A:188:GLU:N	2.41	0.52
1:B:56:LEU:HA	1:B:86:LEU:HD13	1.92	0.52
1:A:335:VAL:HG11	1:A:347:ILE:HD11	1.92	0.52
1:B:334:HIS:HB3	1:B:372:ALA:HB1	1.91	0.51
1:A:395:ILE:HG21	1:A:402:ILE:HG21	1.93	0.51
1:B:1:MET:H3	1:B:419:GLU:HB2	1.75	0.51
1:A:137:LYS:NZ	1:A:142:TYR:OH	2.24	0.51
1:B:40:GLU:HB3	1:B:225:VAL:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:HG22	3:A:487:HOH:O	2.10	0.51
1:B:126:ILE:HG23	1:B:136:ILE:HG21	1.91	0.51
1:A:89:THR:CG2	3:A:554:HOH:O	2.56	0.50
1:B:152:LYS:N	1:B:152:LYS:HD3	2.25	0.50
1:B:263:LEU:HD12	3:B:575:HOH:O	2.10	0.50
1:A:332:PHE:CE1	1:A:352:VAL:HG23	2.47	0.50
2:A:479:HAI:H41	2:A:480:HAI:C4	2.38	0.50
1:A:64:VAL:HG13	1:A:72:ILE:HD13	1.93	0.50
1:A:31:ALA:HB1	1:A:198:LEU:HD21	1.93	0.49
1:A:334:HIS:HD2	3:A:512:HOH:O	1.95	0.49
1:B:309:GLN:H	1:B:309:GLN:NE2	2.10	0.49
1:B:299:HIS:CG	1:B:300:PRO:HA	2.48	0.49
1:A:63:LYS:CE	1:A:76:ASN:HD22	2.26	0.48
1:B:120:ARG:HB2	1:B:123:ASP:OD2	2.14	0.48
1:B:370:LEU:HD23	1:B:395:ILE:HA	1.96	0.48
1:A:299:HIS:CG	1:A:300:PRO:HA	2.49	0.47
1:A:66:ARG:HG3	1:A:70:VAL:HG22	1.96	0.47
1:A:335:VAL:HG21	1:A:347:ILE:HD11	1.96	0.47
1:B:125:HIS:HD2	1:B:168:THR:OG1	1.96	0.47
1:B:315:LEU:HD21	1:B:345:ALA:HB2	1.96	0.47
1:B:83:PRO:HG2	1:B:86:LEU:HG	1.94	0.47
1:A:267:ARG:HG3	1:A:273:ILE:HD12	1.95	0.47
1:A:91:ARG:HH11	1:A:91:ARG:CG	2.22	0.47
1:A:329:GLU:HA	3:A:665:HOH:O	2.14	0.47
1:A:359:LYS:HD2	1:A:384:GLU:OE2	2.14	0.47
1:B:83:PRO:HD2	1:B:86:LEU:CD1	2.38	0.46
1:B:232:ARG:O	1:B:259:LEU:HD21	2.15	0.46
2:A:480:HAI:C5	1:B:250:VAL:HG11	2.45	0.46
1:B:287:LYS:HE2	3:B:463:HOH:O	2.14	0.46
1:A:157:VAL:HA	1:A:183:GLU:HB2	1.97	0.46
1:A:295:ARG:NH1	1:A:326:THR:HG21	2.31	0.46
1:A:288:ARG:CG	1:A:289:PRO:HD2	2.46	0.45
1:B:39:VAL:HG12	1:B:223:GLY:HA2	1.98	0.45
1:A:392:ILE:HD12	1:A:392:ILE:HA	1.63	0.45
1:A:264:ALA:O	1:A:268:GLU:HG3	2.17	0.45
1:A:403:GLU:O	1:A:407:ARG:HB2	2.17	0.45
1:A:13:GLN:HA	1:A:248:LYS:O	2.17	0.45
1:A:91:ARG:O	1:A:94:ILE:HG22	2.17	0.45
1:A:5:ARG:HH11	1:A:5:ARG:HG3	1.81	0.45
1:B:5:ARG:NH1	1:B:386:THR:HG21	2.32	0.45
1:B:87:VAL:HB	1:B:93:SER:OG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:GLU:O	1:B:407:ARG:HB2	2.16	0.45
1:A:109:VAL:HG12	1:A:110:SER:O	2.18	0.44
1:A:21:ALA:HB2	1:A:231:ASP:HA	2.00	0.44
1:B:317:ALA:O	1:B:356:GLY:HA3	2.17	0.44
1:A:303:PRO:HG2	1:A:306:MET:HB2	2.00	0.44
1:B:370:LEU:CD2	1:B:395:ILE:HA	2.48	0.44
1:A:137:LYS:HB3	1:A:144:LYS:HB3	1.99	0.44
1:B:139:GLU:O	1:B:140:GLU:C	2.56	0.44
1:A:325:GLU:HG3	1:A:328:PHE:O	2.17	0.43
1:A:329:GLU:CA	3:A:665:HOH:O	2.66	0.43
1:A:128:GLY:HA3	1:A:169:ILE:HD11	2.00	0.43
1:A:120:ARG:HA	1:A:120:ARG:HE	1.82	0.43
1:A:267:ARG:HH11	1:A:267:ARG:HD2	1.44	0.43
1:A:276:GLY:HA3	1:A:279:TRP:NE1	2.33	0.43
1:B:299:HIS:CD2	1:B:300:PRO:HA	2.53	0.43
1:B:85:ASP:HA	1:B:88:LYS:HD3	1.99	0.43
1:A:3:LYS:HB2	1:A:416:VAL:HG22	2.00	0.43
1:A:101:VAL:HG11	1:A:145:ALA:CB	2.45	0.43
1:A:36:GLU:O	1:A:75:SER:HB3	2.19	0.43
1:A:83:PRO:O	1:A:87:VAL:HG13	2.18	0.43
1:B:124:LEU:HD11	1:B:160:LYS:CG	2.49	0.43
1:B:333:MET:HG3	3:B:531:HOH:O	2.19	0.43
1:B:116:ALA:O	1:B:120:ARG:HD3	2.19	0.42
1:A:12:LEU:O	1:A:247:GLY:HA3	2.19	0.42
1:A:265:LYS:HB3	1:A:310:PHE:CE2	2.55	0.42
1:B:359:LYS:O	3:B:611:HOH:O	2.21	0.42
1:B:389:VAL:CG1	1:B:392:ILE:HD11	2.49	0.42
1:A:320:THR:OG1	1:A:355:HIS:HD2	2.02	0.42
1:B:63:LYS:CE	1:B:65:GLU:HG3	2.50	0.42
1:A:41:ILE:O	1:A:69:SER:HA	2.20	0.42
1:A:348:GLU:O	1:A:349:SER:HB3	2.19	0.42
1:A:391:ARG:NH1	1:A:394:HIS:HE1	2.18	0.42
1:A:7:GLN:HG2	1:A:386:THR:OG1	2.19	0.42
1:A:153:GLY:HA2	1:A:180:THR:OG1	2.20	0.42
1:A:295:ARG:CZ	1:A:326:THR:HG21	2.50	0.42
1:A:335:VAL:CB	1:A:336:PRO:HD3	2.44	0.42
1:A:139:GLU:HB2	1:A:142:TYR:CZ	2.54	0.41
1:A:179:THR:HA	1:A:215:ILE:O	2.20	0.41
1:B:83:PRO:O	1:B:87:VAL:HG13	2.19	0.41
1:B:152:LYS:HD3	1:B:152:LYS:H	1.83	0.41
1:B:297:ALA:HB1	1:B:298:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LYS:HE2	1:A:76:ASN:HD22	1.85	0.41
1:B:159:ASP:OD1	1:B:160:LYS:HG2	2.20	0.41
1:A:249:ILE:HD13	1:A:249:ILE:HG21	1.89	0.41
1:B:413:ILE:HG21	1:B:413:ILE:HD13	1.73	0.41
1:A:86:LEU:HB3	3:A:612:HOH:O	2.21	0.41
1:A:279:TRP:CH2	2:A:479:HAI:H22	2.56	0.41
1:A:3:LYS:HG2	1:A:390:ASP:OD1	2.20	0.41
1:A:9:PRO:HD3	1:A:384:GLU:OE1	2.20	0.41
1:A:59:GLN:HG2	1:A:86:LEU:HD12	2.03	0.41
1:A:334:HIS:CD2	3:A:512:HOH:O	2.71	0.41
1:B:3:LYS:HG2	1:B:390:ASP:HA	2.03	0.41
1:B:320:THR:HA	1:B:354:CYS:O	2.20	0.41
1:A:5:ARG:HD2	1:A:7:GLN:HE21	1.86	0.40
1:B:53:THR:O	1:B:57:LEU:HG	2.21	0.40
1:A:227:ARG:HH11	1:A:227:ARG:HD2	1.56	0.40
1:B:335:VAL:HG22	1:B:347:ILE:CD1	2.36	0.40
1:B:30:PHE:HE1	1:B:56:LEU:HD22	1.86	0.40
1:B:111:LEU:HA	1:B:112:PRO:HD3	1.84	0.40
1:A:4:PHE:CD2	1:A:392:ILE:HG13	2.57	0.40
1:A:197:PHE:O	1:A:200:ALA:HB3	2.21	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:642:HOH:O	3:B:491:HOH:O[3_455]	0.49	1.71
3:A:692:HOH:O	3:B:535:HOH:O[3_455]	2.19	0.01

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	417/419 (100%)	407 (98%)	8 (2%)	2 (0%)	29	23
1	B	417/419 (100%)	406 (97%)	8 (2%)	3 (1%)	22	16
All	All	834/838 (100%)	813 (98%)	16 (2%)	5 (1%)	25	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	B	67	ASN
1	A	68	GLY
1	B	119	ALA
1	B	121	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/330 (100%)	312 (94%)	18 (6%)	21	17
1	B	330/330 (100%)	306 (93%)	24 (7%)	14	9
All	All	660/660 (100%)	618 (94%)	42 (6%)	17	13

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	66	ARG
1	A	67	ASN
1	A	76	ASN
1	A	91	ARG
1	A	101	VAL
1	A	120	ARG
1	A	131	LYS
1	A	148	ASN
1	A	160	LYS
1	A	220	ARG

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Mol	Chain	Res	Type
1	A	229	LEU
1	A	307	GLN
1	A	322	VAL
1	A	360	LEU
1	A	370	LEU
1	A	392	ILE
1	A	412	ASN
1	B	55	LYS
1	B	65	GLU
1	B	66	ARG
1	B	86	LEU
1	B	88	LYS
1	B	91	ARG
1	B	110	SER
1	B	126	ILE
1	B	131	LYS
1	B	137	LYS
1	B	150	ARG
1	B	152	LYS
1	B	160	LYS
1	B	175	LEU
1	B	210	THR
1	B	229	LEU
1	B	248	LYS
1	B	292	VAL
1	B	309	GLN
1	B	370	LEU
1	B	375	SER
1	B	378	LEU
1	B	392	ILE
1	B	412	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	59	GLN
1	A	67	ASN
1	A	76	ASN
1	A	79	ASN
1	A	125	HIS
1	A	155	HIS

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	299	HIS
1	A	334	HIS
1	A	355	HIS
1	A	394	HIS
1	A	412	ASN
1	B	7	GLN
1	B	125	HIS
1	B	148	ASN
1	B	155	HIS
1	B	285	HIS
1	B	299	HIS
1	B	309	GLN
1	B	355	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are 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	HAI	A	479	-	7,7,7	1.93	2 (28%)	8,8,8	6.65	5 (62%)
2	HAI	A	480	-	7,7,7	1.50	1 (14%)	8,8,8	9.86	5 (62%)

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	HAI	A	479	-	-	-	0/1/1/1
2	HAI	A	480	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	479	HAI	C5-C6	3.97	1.63	1.53
2	A	480	HAI	C5-C6	-3.57	1.44	1.53
2	A	479	HAI	C2-C1	-2.76	1.43	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	480	HAI	C6-C1-C2	-23.78	86.10	110.29
2	A	479	HAI	C6-C1-C2	16.70	127.27	110.29
2	A	480	HAI	C4-C5-C6	-10.98	88.86	111.42
2	A	480	HAI	C5-C6-C1	8.06	122.69	111.77
2	A	479	HAI	C4-C5-C6	6.91	125.62	111.42
2	A	480	HAI	C3-C2-C1	-4.24	106.03	111.77
2	A	479	HAI	C5-C6-C1	-3.90	106.48	111.77
2	A	480	HAI	C5-C4-C3	2.48	118.56	111.19
2	A	479	HAI	C5-C4-C3	-2.45	103.93	111.19
2	A	479	HAI	C2-C1-N	2.02	117.19	111.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	479	HAI	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	480	HAI	6	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.