



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:31 PM UTC

PDB ID : 1YPP / pdb_00001ypp
Title : ACID ANHYDRIDE HYDROLASE
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Deposited on : 1996-05-29
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

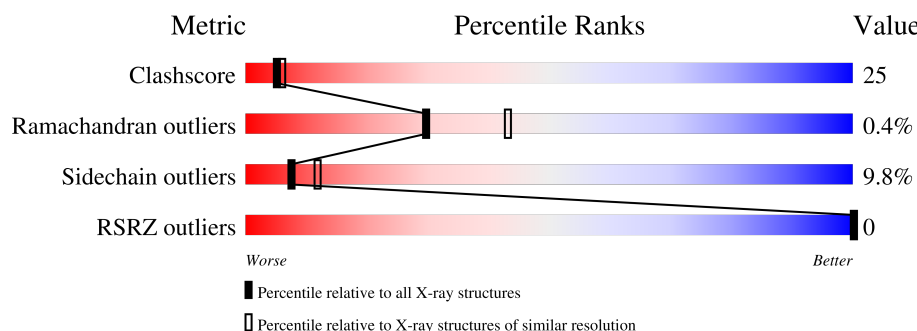
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	286	
1	B	286	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4746 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 INORGANIC PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2248	1444	369	432	3			
1	B	282	Total	C	N	O	S	0	0	0
			2248	1444	369	432	3			

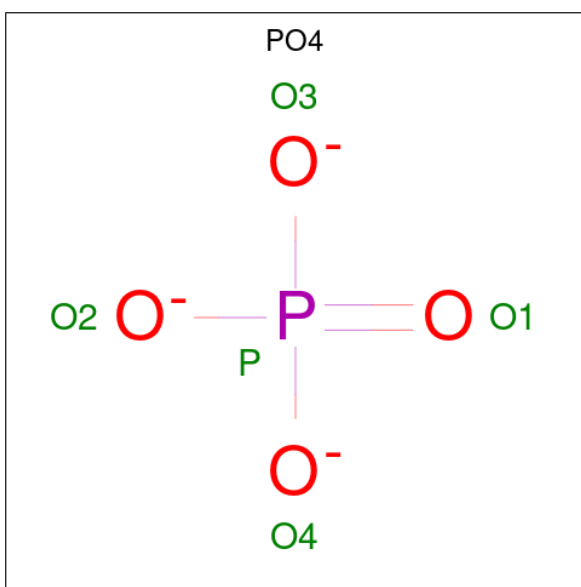
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	ALA	LYS	conflict	UNP P00817
A	266	PRO	LEU	conflict	UNP P00817
B	73	ALA	LYS	conflict	UNP P00817
B	266	PRO	LEU	conflict	UNP P00817

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Mn	0	0
			4	4		
2	B	4	Total	Mn	0	0
			4	4		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

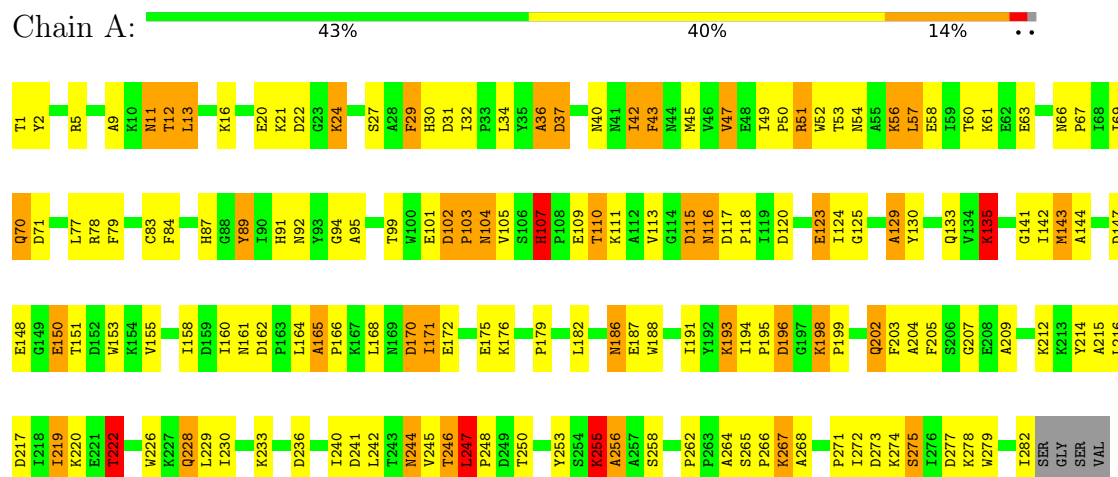
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	112	Total	O	0	0
			112	112		

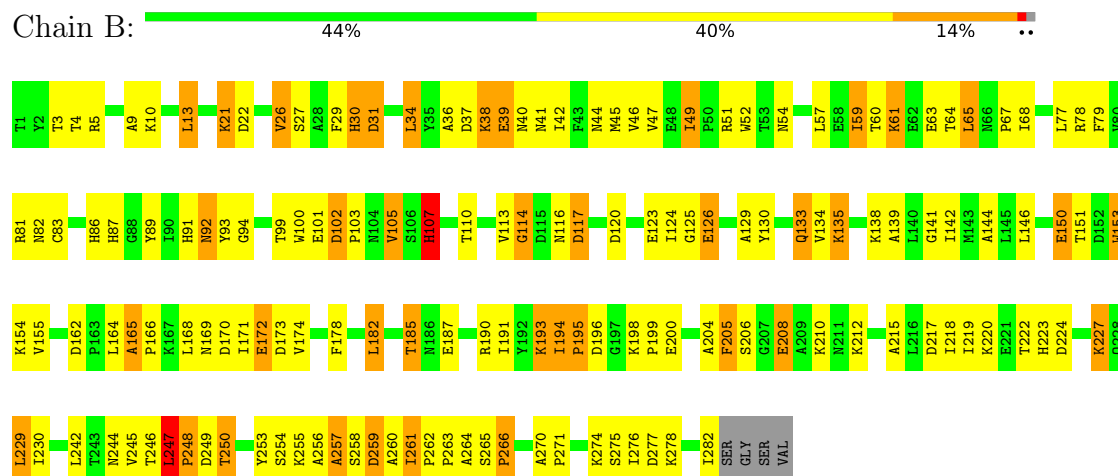
3 Residue-property plots

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 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: INORGANIC PYROPHOSPHATASE



• Molecule 1: INORGANIC PYROPHOSPHATASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.00Å 106.20Å 56.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	79.0 (10.00-2.40) 77.9 (10.00-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.35 (at 2.41Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available) 0.166 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.926	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4746	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MN

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	1.45	16/2307 (0.7%)	2.14	97/3139 (3.1%)
1	B	1.42	13/2307 (0.6%)	2.08	81/3139 (2.6%)
All	All	1.44	29/4614 (0.6%)	2.11	178/6278 (2.8%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	194	ILE	CA-CB	-8.09	1.48	1.53
1	B	49	ILE	CA-CB	7.82	1.61	1.54
1	A	111	LYS	N-CA	7.26	1.55	1.46
1	B	191	ILE	CA-CB	7.22	1.62	1.54
1	B	124	ILE	N-CA	-7.21	1.37	1.46
1	A	66	ASN	CA-CB	7.03	1.58	1.52
1	B	92	ASN	CA-CB	-6.97	1.42	1.53
1	A	92	ASN	N-CA	6.74	1.54	1.46
1	A	92	ASN	CA-CB	-6.62	1.42	1.53
1	A	110	THR	C-O	6.49	1.32	1.23
1	A	124	ILE	N-CA	-6.37	1.38	1.46
1	B	141	GLY	N-CA	6.29	1.51	1.45
1	B	94	GLY	N-CA	5.62	1.53	1.45
1	A	101	GLU	N-CA	5.47	1.53	1.46
1	A	110	THR	C-N	-5.43	1.26	1.33
1	A	110	THR	N-CA	5.43	1.52	1.45
1	B	150	GLU	N-CA	-5.35	1.39	1.46
1	B	30	HIS	CA-CB	5.32	1.62	1.53
1	B	134	VAL	N-CA	5.31	1.53	1.46
1	B	57	LEU	CA-CB	-5.27	1.44	1.53
1	B	191	ILE	N-CA	-5.26	1.39	1.46
1	A	53	THR	N-CA	-5.20	1.39	1.45
1	A	31	ASP	N-CA	-5.17	1.39	1.46
1	A	94	GLY	N-CA	5.15	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49	ILE	CA-CB	5.06	1.60	1.54
1	A	198	LYS	CA-CB	-5.04	1.45	1.53
1	A	150	GLU	N-CA	-5.03	1.39	1.45
1	A	255	LYS	N-CA	5.02	1.52	1.45
1	B	61	LYS	N-CA	-5.01	1.40	1.46

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ARG	CD-NE-CZ	18.48	150.27	124.40
1	A	117	ASP	CA-CB-CG	14.46	127.06	112.60
1	B	117	ASP	CA-CB-CG	14.37	126.97	112.60
1	A	110	THR	CA-C-O	-12.41	107.08	121.72
1	A	37	ASP	CA-CB-CG	12.32	124.92	112.60
1	B	191	ILE	N-CA-C	11.14	123.60	112.90
1	B	92	ASN	CA-CB-CG	10.97	123.57	112.60
1	B	29	PHE	CA-CB-CG	10.77	124.57	113.80
1	A	116	ASN	OD1-CG-ND2	-10.09	112.51	122.60
1	A	70	GLN	OE1-CD-NE2	9.71	132.31	122.60
1	A	29	PHE	CA-CB-CG	9.52	123.32	113.80
1	A	92	ASN	CA-CB-CG	9.05	121.65	112.60
1	B	82	ASN	OD1-CG-ND2	-8.75	113.85	122.60
1	A	92	ASN	CA-C-O	-8.66	111.46	121.16
1	B	39	GLU	CA-C-N	8.38	135.81	121.14
1	B	39	GLU	C-N-CA	8.38	135.81	121.14
1	A	277	ASP	CA-CB-CG	8.28	120.88	112.60
1	A	110	THR	N-CA-C	-8.26	98.30	110.52
1	B	229	LEU	N-CA-C	8.14	119.84	110.97
1	B	170	ASP	CA-CB-CG	8.13	120.73	112.60
1	A	91	HIS	CA-C-O	-8.07	111.95	120.99
1	A	255	LYS	N-CA-C	-7.90	99.89	110.55
1	B	116	ASN	OD1-CG-ND2	-7.83	114.77	122.60
1	A	54	ASN	CA-CB-CG	7.80	120.40	112.60
1	A	120	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	116	ASN	CA-CB-CG	7.70	120.30	112.60
1	B	247	LEU	CA-C-N	7.58	127.22	119.56
1	B	247	LEU	C-N-CA	7.58	127.22	119.56
1	B	107	HIS	CA-C-N	7.52	127.23	119.56
1	B	107	HIS	C-N-CA	7.52	127.23	119.56
1	A	217	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	236	ASP	CA-CB-CG	7.20	119.80	112.60
1	A	165	ALA	CA-C-N	7.06	128.66	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ALA	C-N-CA	7.06	128.66	119.84
1	A	172	GLU	CB-CG-CD	6.99	124.48	112.60
1	A	171	ILE	N-CA-C	6.92	117.68	110.62
1	B	254	SER	N-CA-C	6.91	119.37	107.28
1	B	266	PRO	N-CA-CB	6.86	109.37	103.19
1	B	190	ARG	NE-CZ-NH2	6.80	125.32	119.20
1	B	191	ILE	CB-CA-C	-6.73	102.85	111.20
1	A	102	ASP	CA-C-N	6.73	126.18	118.85
1	A	102	ASP	C-N-CA	6.73	126.18	118.85
1	A	52	TRP	CA-C-N	6.71	133.12	122.59
1	A	52	TRP	C-N-CA	6.71	133.12	122.59
1	B	250	THR	N-CA-CB	6.70	121.17	110.11
1	B	259	ASP	CA-CB-CG	6.69	119.29	112.60
1	A	71	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	12	THR	N-CA-CB	6.66	120.72	110.60
1	A	198	LYS	N-CA-CB	6.65	117.31	109.72
1	A	247	LEU	CA-C-N	6.64	126.34	119.64
1	A	247	LEU	C-N-CA	6.64	126.34	119.64
1	B	31	ASP	CA-CB-CG	-6.62	105.98	112.60
1	A	135	LYS	CA-CB-CG	6.61	127.33	114.10
1	A	170	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	250	THR	CA-C-N	6.60	126.38	119.05
1	A	250	THR	C-N-CA	6.60	126.38	119.05
1	B	165	ALA	CA-C-N	6.59	127.11	119.47
1	B	165	ALA	C-N-CA	6.59	127.11	119.47
1	B	92	ASN	N-CA-C	-6.56	99.33	109.76
1	B	102	ASP	CA-CB-CG	6.54	119.14	112.60
1	B	49	ILE	CB-CA-C	-6.50	103.30	110.52
1	B	83	CYS	CA-C-O	-6.50	113.58	120.40
1	B	135	LYS	CA-CB-CG	6.50	127.09	114.10
1	B	205	PHE	CA-CB-CG	6.45	120.25	113.80
1	A	107	HIS	CA-C-N	6.44	126.36	119.28
1	A	107	HIS	C-N-CA	6.44	126.36	119.28
1	A	110	THR	CA-C-N	-6.43	112.86	122.24
1	A	110	THR	C-N-CA	-6.43	112.86	122.24
1	A	49	ILE	N-CA-CB	-6.39	102.27	111.21
1	B	139	ALA	CA-C-O	-6.39	114.17	121.19
1	B	102	ASP	CA-C-N	6.37	125.79	118.85
1	B	102	ASP	C-N-CA	6.37	125.79	118.85
1	A	103	PRO	CA-C-N	6.35	134.64	121.94
1	A	103	PRO	C-N-CA	6.35	134.64	121.94
1	A	51	ARG	CB-CG-CD	6.30	125.79	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	HIS	N-CA-C	6.29	121.48	113.55
1	B	79	PHE	CA-CB-CG	6.25	120.05	113.80
1	A	219	ILE	CA-CB-CG1	6.14	120.85	110.40
1	B	257	ALA	N-CA-C	-6.11	104.70	111.36
1	A	92	ASN	N-CA-C	-6.11	101.24	110.28
1	A	279	TRP	CA-CB-CG	6.09	125.17	113.60
1	B	133	GLN	CA-C-N	-6.07	115.28	122.93
1	B	133	GLN	C-N-CA	-6.07	115.28	122.93
1	A	191	ILE	N-CA-C	6.05	121.37	113.07
1	B	261	ILE	CA-C-N	6.00	126.56	120.38
1	B	261	ILE	C-N-CA	6.00	126.56	120.38
1	A	124	ILE	N-CA-C	5.99	121.80	109.34
1	A	78	ARG	CA-C-N	5.98	132.38	122.33
1	A	78	ARG	C-N-CA	5.98	132.38	122.33
1	A	89	TYR	O-C-N	-5.96	115.59	122.93
1	B	51	ARG	CB-CG-CD	5.88	124.83	111.30
1	A	123	GLU	CA-C-N	5.86	132.51	121.97
1	A	123	GLU	C-N-CA	5.86	132.51	121.97
1	A	205	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	47	VAL	N-CA-CB	5.81	117.06	110.72
1	A	116	ASN	CA-CB-CG	5.80	118.40	112.60
1	B	271	PRO	N-CA-CB	5.80	108.72	103.33
1	A	89	TYR	CB-CA-C	5.79	119.16	109.89
1	B	30	HIS	CA-CB-CG	-5.72	108.08	113.80
1	B	92	ASN	N-CA-CB	5.72	118.82	109.95
1	A	66	ASN	CA-C-N	5.70	126.02	119.92
1	A	66	ASN	C-N-CA	5.70	126.02	119.92
1	A	78	ARG	NE-CZ-NH1	-5.70	115.80	121.50
1	B	36	ALA	N-CA-C	-5.69	106.50	113.50
1	B	194	ILE	CA-C-N	5.69	126.95	119.84
1	B	194	ILE	C-N-CA	5.69	126.95	119.84
1	A	104	ASN	N-CA-C	5.67	120.06	113.20
1	A	244	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	219	ILE	N-CA-CB	5.67	116.80	110.51
1	A	222	THR	N-CA-CB	-5.66	101.50	110.22
1	B	257	ALA	CA-C-N	5.66	128.43	120.28
1	B	257	ALA	C-N-CA	5.66	128.43	120.28
1	A	233	LYS	N-CA-C	5.65	119.80	113.02
1	B	49	ILE	CA-C-N	5.62	125.59	120.03
1	B	49	ILE	C-N-CA	5.62	125.59	120.03
1	B	63	GLU	N-CA-CB	5.60	119.80	110.85
1	A	220	LYS	N-CA-C	5.58	117.36	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	LEU	CA-CB-CG	5.57	135.81	116.30
1	A	162	ASP	CA-C-N	5.56	126.80	119.84
1	A	162	ASP	C-N-CA	5.56	126.80	119.84
1	B	248	PRO	N-CA-CB	5.55	108.84	103.51
1	B	259	ASP	N-CA-C	-5.55	106.35	113.23
1	B	217	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	126	GLU	CB-CG-CD	5.54	122.01	112.60
1	B	250	THR	CA-C-N	5.50	124.96	119.24
1	B	250	THR	C-N-CA	5.50	124.96	119.24
1	A	255	LYS	CA-C-O	-5.47	115.36	121.81
1	A	50	PRO	N-CA-CB	5.45	108.52	103.39
1	B	5	ARG	CD-NE-CZ	5.44	132.01	124.40
1	A	42	ILE	N-CA-CB	5.43	118.75	111.90
1	A	150	GLU	CB-CG-CD	-5.42	103.39	112.60
1	A	102	ASP	O-C-N	5.42	127.55	121.32
1	B	208	GLU	CB-CG-CD	5.41	121.80	112.60
1	A	196	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	190	ARG	CA-CB-CG	5.38	124.85	114.10
1	B	258	SER	N-CA-C	5.37	117.89	111.71
1	A	16	LYS	CA-CB-CG	5.36	124.81	114.10
1	A	198	LYS	CA-CB-CG	5.32	124.74	114.10
1	A	12	THR	CA-CB-OG1	5.32	117.57	109.60
1	B	44	ASN	OD1-CG-ND2	5.30	127.90	122.60
1	A	186	ASN	N-CA-C	-5.29	105.43	111.14
1	A	196	ASP	N-CA-C	-5.29	106.51	113.17
1	A	135	LYS	CB-CA-C	5.26	119.87	109.66
1	A	32	ILE	N-CA-C	-5.26	101.73	107.73
1	B	36	ALA	CA-C-N	5.24	129.06	121.26
1	B	36	ALA	C-N-CA	5.24	129.06	121.26
1	A	271	PRO	N-CA-CB	5.24	108.20	103.33
1	A	66	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	123	GLU	O-C-N	-5.23	116.65	122.93
1	A	262	PRO	N-CA-CB	5.23	108.16	103.08
1	A	49	ILE	CA-C-N	5.22	125.51	119.92
1	A	49	ILE	C-N-CA	5.22	125.51	119.92
1	A	198	LYS	N-CA-C	-5.22	104.05	110.31
1	A	11	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	B	153	TRP	CA-C-N	-5.21	115.75	123.05
1	B	153	TRP	C-N-CA	-5.21	115.75	123.05
1	A	36	ALA	N-CA-C	-5.21	106.61	113.12
1	A	79	PHE	CA-CB-CG	5.21	119.00	113.80
1	B	120	ASP	CA-CB-CG	5.20	117.80	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ALA	CA-C-O	-5.17	116.04	121.88
1	A	268	ALA	CB-CA-C	5.16	118.96	109.46
1	B	185	THR	CA-C-N	5.14	127.12	120.44
1	B	185	THR	C-N-CA	5.14	127.12	120.44
1	B	78	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	B	218	ILE	CA-C-O	-5.13	115.62	120.95
1	B	162	ASP	CA-CB-CG	-5.11	107.49	112.60
1	B	270	ALA	CA-C-N	5.11	125.01	119.85
1	B	270	ALA	C-N-CA	5.11	125.01	119.85
1	B	114	GLY	N-CA-C	-5.10	104.64	112.85
1	A	32	ILE	CA-C-N	5.10	125.33	119.83
1	A	32	ILE	C-N-CA	5.10	125.33	119.83
1	B	263	PRO	N-CA-CB	5.08	108.16	103.39
1	B	45	MET	CA-C-N	-5.07	116.42	122.90
1	B	45	MET	C-N-CA	-5.07	116.42	122.90
1	A	179	PRO	N-CA-CB	5.06	107.67	103.17
1	A	161	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	56	LYS	O-C-N	5.03	128.45	122.46
1	A	43	PHE	CA-CB-CG	5.03	118.83	113.80

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	2248	0	2218	111	0
1	B	2248	0	2218	110	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	110	0	0	13	0
4	B	112	0	0	14	0
All	All	4746	0	4436	220	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (220) 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:99:THR:HB	1:A:222:THR:CG2	1.88	1.02
1:A:99:THR:HB	1:A:222:THR:HG23	1.46	0.98
1:B:215:ALA:O	1:B:219:ILE:HD12	1.64	0.97
1:B:99:THR:HB	1:B:222:THR:CG2	1.96	0.94
1:B:224:ASP:HA	1:B:227:LYS:HD3	1.56	0.87
1:B:150:GLU:OE1	4:B:437:HOH:O	1.93	0.86
1:A:45:MET:HE2	1:A:47:VAL:HG22	1.57	0.86
1:A:247:LEU:O	1:A:253:TYR:HB2	1.79	0.82
1:A:70:GLN:CB	4:A:440:HOH:O	2.29	0.80
1:A:42:ILE:HD13	1:A:160:ILE:HG21	1.65	0.79
1:A:129:ALA:HB1	1:A:133:GLN:NE2	1.97	0.78
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.65	0.78
1:A:175:GLU:OE1	4:A:436:HOH:O	2.02	0.77
1:A:30:HIS:HD2	1:A:226:TRP:HE1	1.34	0.75
1:B:99:THR:HB	1:B:222:THR:HG22	1.69	0.74
1:B:282:ILE:HG22	1:B:282:ILE:O	1.87	0.73
1:A:36:ALA:HB3	1:A:42:ILE:HG22	1.69	0.73
1:B:59:ILE:HG13	1:B:68:ILE:HG12	1.69	0.73
1:A:130:TYR:CE1	1:A:133:GLN:HG3	2.22	0.73
1:A:274:LYS:N	1:A:274:LYS:HD2	2.03	0.73
1:A:13:LEU:HD13	1:A:77:LEU:HD21	1.70	0.73
1:A:202:GLN:NE2	4:A:481:HOH:O	2.16	0.72
1:B:196:ASP:OD2	4:B:483:HOH:O	2.06	0.72
1:A:274:LYS:HD2	1:A:274:LYS:H	1.54	0.71
1:A:147:ASP:O	4:A:411:HOH:O	2.10	0.70
1:A:195:PRO:HG3	1:A:282:ILE:HD11	1.74	0.69
1:B:130:TYR:H	1:B:133:GLN:HE21	1.41	0.69
1:A:70:GLN:HB3	4:A:440:HOH:O	1.89	0.68
1:A:109:GLU:HG2	1:A:214:TYR:OH	1.94	0.67
1:B:105:VAL:O	1:B:113:VAL:HA	1.93	0.67
1:A:51:ARG:NH1	4:A:406:HOH:O	2.26	0.66
1:A:142:ILE:HG12	1:A:153:TRP:CE3	2.30	0.66
1:B:126:GLU:OE1	4:B:476:HOH:O	2.13	0.66
1:A:255:LYS:NZ	1:A:258:SER:HB2	2.10	0.66
1:B:102:ASP:HB3	1:B:105:VAL:HG23	1.77	0.66
1:A:141:GLY:HA3	1:A:171:ILE:HD13	1.77	0.66
1:A:202:GLN:N	1:A:202:GLN:HE21	1.93	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:HG22	1:B:210:LYS:HB2	1.77	0.65
1:B:54:ASN:OD1	4:B:433:HOH:O	2.14	0.65
1:A:133:GLN:NE2	1:A:135:LYS:HE3	2.12	0.65
1:A:215:ALA:O	1:A:219:ILE:HD12	1.97	0.64
1:A:129:ALA:HB1	1:A:133:GLN:HE22	1.62	0.64
1:B:31:ASP:OD2	1:B:245:VAL:HG22	1.96	0.64
1:B:255:LYS:O	1:B:256:ALA:HB3	1.98	0.64
1:B:276:ILE:O	4:B:408:HOH:O	2.15	0.64
1:A:255:LYS:O	1:A:256:ALA:HB3	1.97	0.63
1:B:40:ASN:O	1:B:41:ASN:HB2	1.98	0.63
1:B:257:ALA:O	1:B:260:ALA:HB3	1.98	0.63
1:B:230:ILE:HG13	1:B:250:THR:HG21	1.81	0.63
1:A:61:LYS:HD2	1:A:240:ILE:HG12	1.80	0.62
1:A:99:THR:HB	1:A:222:THR:HG22	1.80	0.62
1:B:253:TYR:OH	1:B:255:LYS:HG3	2.00	0.62
1:B:99:THR:CB	1:B:222:THR:HG22	2.29	0.61
1:A:13:LEU:HD13	1:A:77:LEU:CD2	2.30	0.61
1:B:144:ALA:HB2	1:B:153:TRP:CZ3	2.36	0.61
1:B:194:ILE:HD11	1:B:200:GLU:HB2	1.83	0.61
1:B:60:THR:HG22	1:B:67:PRO:O	2.01	0.61
1:B:99:THR:HB	1:B:222:THR:HG21	1.83	0.61
1:A:255:LYS:O	1:A:256:ALA:CB	2.49	0.60
1:B:174:VAL:HG11	1:B:182:LEU:HD13	1.82	0.60
1:B:130:TYR:H	1:B:133:GLN:NE2	1.99	0.60
1:B:130:TYR:CE1	1:B:133:GLN:HB2	2.37	0.60
1:A:273:ASP:OD2	1:A:275:SER:OG	2.19	0.60
1:A:123:GLU:OE2	1:A:125:GLY:N	2.33	0.59
1:A:21:LYS:HD2	4:A:459:HOH:O	2.03	0.58
1:A:60:THR:HG22	1:A:67:PRO:O	2.03	0.58
1:A:147:ASP:O	1:A:148:GLU:HB2	2.02	0.58
1:B:142:ILE:HD12	1:B:155:VAL:HG22	1.86	0.58
1:A:202:GLN:HE21	1:A:202:GLN:H	1.51	0.58
1:A:248:PRO:HA	1:A:253:TYR:CG	2.38	0.58
1:A:255:LYS:HZ1	1:A:258:SER:HB2	1.68	0.57
1:A:30:HIS:CD2	1:A:226:TRP:HE1	2.18	0.57
1:A:158:ILE:HD13	1:A:168:LEU:HD12	1.85	0.57
1:B:61:LYS:CE	4:B:450:HOH:O	2.49	0.56
1:B:110:THR:HB	1:B:146:LEU:HD21	1.88	0.56
1:A:57:LEU:O	4:A:413:HOH:O	2.18	0.56
1:B:125:GLY:HA3	4:B:454:HOH:O	2.05	0.56
1:B:168:LEU:HD23	1:B:173:ASP:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ILE:HD12	1:B:242:LEU:HB3	1.87	0.55
1:A:2:TYR:HA	1:A:20:GLU:O	2.06	0.55
1:A:99:THR:CB	1:A:222:THR:CG2	2.75	0.55
1:A:142:ILE:HG12	1:A:153:TRP:HE3	1.72	0.55
1:A:30:HIS:CE1	1:A:242:LEU:HA	2.42	0.54
1:A:37:ASP:CG	1:A:40:ASN:HD22	2.15	0.54
1:A:198:LYS:HB3	1:A:199:PRO:CD	2.38	0.54
1:B:21:LYS:O	1:B:22:ASP:C	2.51	0.54
1:A:129:ALA:CB	1:A:133:GLN:HE22	2.21	0.53
1:A:150:GLU:OE1	4:A:434:HOH:O	2.18	0.53
1:B:101:GLU:OE2	4:B:448:HOH:O	2.18	0.53
1:B:265:SER:N	1:B:266:PRO:CD	2.71	0.53
1:B:230:ILE:HA	1:B:242:LEU:HD13	1.91	0.53
1:B:21:LYS:HB2	1:B:26:VAL:HG11	1.89	0.53
1:B:100:TRP:CZ3	1:B:229:LEU:HD13	2.44	0.53
1:B:49:ILE:HG21	1:B:89:TYR:CD2	2.44	0.53
1:B:102:ASP:OD1	1:B:103:PRO:HD2	2.10	0.52
1:B:130:TYR:CZ	1:B:133:GLN:HB2	2.44	0.52
1:A:99:THR:CG2	1:A:222:THR:HG22	2.39	0.52
1:A:170:ASP:OD1	1:A:212:LYS:HB3	2.10	0.52
1:A:5:ARG:HG3	1:A:264:ALA:HB2	1.91	0.52
1:B:93:TYR:OH	1:B:154:LYS:NZ	2.42	0.52
1:B:13:LEU:HD13	1:B:77:LEU:CD2	2.39	0.52
1:B:165:ALA:HB3	1:B:166:PRO:HD3	1.92	0.52
1:B:27:SER:OG	1:B:30:HIS:HB2	2.10	0.51
1:A:102:ASP:OD1	1:A:104:ASN:HB2	2.10	0.51
1:B:61:LYS:NZ	4:B:450:HOH:O	2.10	0.51
1:B:34:LEU:HD12	1:B:223:HIS:CG	2.45	0.51
1:A:24:LYS:HE3	1:A:255:LYS:CE	2.41	0.51
1:B:255:LYS:O	1:B:256:ALA:CB	2.59	0.51
1:A:165:ALA:HB3	1:A:166:PRO:CD	2.40	0.51
1:B:46:VAL:HG11	1:B:59:ILE:HD11	1.93	0.50
1:A:195:PRO:HD3	1:A:282:ILE:HD13	1.93	0.50
1:A:70:GLN:HB2	4:A:440:HOH:O	2.05	0.50
1:A:116:ASN:OD1	1:A:240:ILE:HD11	2.11	0.50
1:B:282:ILE:O	1:B:282:ILE:CG2	2.59	0.50
1:A:24:LYS:HE3	1:A:255:LYS:HE3	1.93	0.50
1:A:58:GLU:CD	4:A:419:HOH:O	2.54	0.50
1:A:241:ASP:OD1	1:A:241:ASP:C	2.54	0.50
1:B:21:LYS:HB2	1:B:26:VAL:CG1	2.42	0.50
1:B:245:VAL:O	1:B:245:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:CYS:O	1:A:84:PHE:C	2.55	0.49
1:B:195:PRO:HD3	1:B:282:ILE:HD11	1.94	0.49
1:A:103:PRO:O	1:A:113:VAL:HB	2.12	0.49
1:A:142:ILE:HD12	1:A:155:VAL:HG22	1.94	0.49
1:B:9:ALA:O	1:B:10:LYS:C	2.55	0.49
1:B:165:ALA:N	1:B:166:PRO:HD2	2.28	0.49
1:B:230:ILE:HG12	1:B:247:LEU:HD23	1.95	0.49
1:A:95:ALA:HB1	1:A:118:PRO:HB2	1.94	0.49
1:A:115:ASP:HB3	1:A:151:THR:O	2.13	0.49
1:B:86:HIS:NE2	1:B:187:GLU:OE2	2.36	0.49
1:A:193:LYS:NZ	3:A:301:PO4:O2	2.35	0.48
1:A:244:ASN:ND2	1:A:247:LEU:HD23	2.28	0.48
1:A:193:LYS:O	1:A:196:ASP:HB2	2.13	0.48
1:A:198:LYS:CB	1:A:199:PRO:CD	2.92	0.48
1:A:202:GLN:NE2	1:A:202:GLN:N	2.60	0.48
1:A:11:ASN:ND2	1:A:272:ILE:HD11	2.29	0.48
1:A:170:ASP:OD1	1:A:212:LYS:CB	2.63	0.47
1:A:202:GLN:NE2	1:A:202:GLN:H	2.13	0.47
1:B:265:SER:N	1:B:266:PRO:HD3	2.28	0.47
1:B:38:LYS:O	1:B:38:LYS:NZ	2.45	0.47
1:A:244:ASN:OD1	1:A:253:TYR:HA	2.14	0.47
1:B:164:LEU:O	1:B:165:ALA:C	2.56	0.46
1:B:123:GLU:OE2	1:B:125:GLY:N	2.43	0.46
1:A:43:PHE:HZ	1:A:216:LEU:CD2	2.28	0.46
1:A:246:THR:O	1:A:248:PRO:HD3	2.15	0.46
1:B:52:TRP:N	1:B:89:TYR:O	2.36	0.46
1:B:194:ILE:N	1:B:195:PRO:CD	2.78	0.46
1:B:247:LEU:O	1:B:253:TYR:HB2	2.16	0.46
1:A:29:PHE:HE1	1:A:99:THR:O	2.00	0.45
1:A:143:MET:HE3	1:A:209:ALA:HB2	1.98	0.45
1:A:133:GLN:HE22	1:A:135:LYS:HE3	1.79	0.45
1:A:107:HIS:CD2	1:A:107:HIS:N	2.84	0.45
1:B:107:HIS:HB3	4:B:430:HOH:O	2.16	0.45
1:B:193:LYS:O	1:B:196:ASP:HB2	2.17	0.45
1:A:165:ALA:CB	1:A:166:PRO:HD3	2.43	0.45
1:A:60:THR:HB	1:A:69:ILE:HG12	1.99	0.45
1:A:187:GLU:O	1:A:188:TRP:C	2.59	0.45
1:B:37:ASP:CG	1:B:40:ASN:HD22	2.25	0.45
1:B:244:ASN:OD1	1:B:253:TYR:HA	2.17	0.45
1:B:277:ASP:O	1:B:278:LYS:C	2.59	0.45
1:B:3:THR:HB	1:B:4:THR:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:HE2	1:A:89:TYR:OH	2.18	0.44
1:B:246:THR:O	1:B:248:PRO:HD3	2.17	0.44
1:B:261:ILE:HA	1:B:262:PRO:HD3	1.89	0.44
1:B:27:SER:HB2	1:B:65:LEU:HD12	1.99	0.44
1:B:91:HIS:NE2	1:B:185:THR:OG1	2.47	0.44
1:B:138:LYS:HE3	4:B:481:HOH:O	2.17	0.44
1:A:265:SER:N	1:A:266:PRO:CD	2.81	0.44
1:B:194:ILE:C	1:B:196:ASP:H	2.24	0.44
1:A:195:PRO:CG	1:A:282:ILE:HD11	2.44	0.44
1:A:245:VAL:HB	1:A:255:LYS:CD	2.47	0.44
1:A:158:ILE:HD13	1:A:168:LEU:CD1	2.48	0.44
1:B:37:ASP:HB3	1:B:42:ILE:HB	2.00	0.44
1:B:103:PRO:O	1:B:113:VAL:HB	2.18	0.44
1:B:256:ALA:HA	1:B:259:ASP:OD1	2.18	0.44
1:B:264:ALA:HB1	1:B:266:PRO:HD3	2.00	0.44
1:A:255:LYS:HZ3	1:A:258:SER:HB2	1.82	0.44
1:B:38:LYS:HZ2	1:B:38:LYS:HG3	1.68	0.44
1:A:195:PRO:HD3	1:A:282:ILE:CD1	2.48	0.44
1:A:229:LEU:HG	1:A:242:LEU:HD21	1.99	0.44
1:B:144:ALA:HB3	1:B:204:ALA:HB3	1.99	0.43
1:A:22:ASP:N	4:A:491:HOH:O	2.50	0.43
1:A:228:GLN:OE1	4:A:451:HOH:O	2.21	0.43
1:B:81:ARG:NH2	1:B:275:SER:O	2.49	0.43
1:B:198:LYS:HA	1:B:199:PRO:HD3	1.82	0.43
1:B:99:THR:CG2	1:B:222:THR:HG22	2.48	0.43
1:B:261:ILE:HG23	1:B:262:PRO:HD2	2.00	0.43
1:A:203:PHE:HB3	1:A:207:GLY:HA2	2.01	0.43
1:B:172:GLU:H	1:B:172:GLU:HG2	1.38	0.43
1:A:229:LEU:CG	1:A:242:LEU:HD21	2.48	0.43
1:B:169:ASN:N	1:B:173:ASP:OD2	2.39	0.43
1:B:174:VAL:O	1:B:178:PHE:HB2	2.18	0.43
1:B:205:PHE:O	1:B:208:GLU:HB2	2.18	0.42
1:A:60:THR:HG23	1:A:63:GLU:HB2	2.01	0.42
1:B:61:LYS:HE2	4:B:450:HOH:O	2.17	0.42
1:A:265:SER:N	1:A:266:PRO:HD3	2.34	0.42
1:B:130:TYR:CD1	1:B:133:GLN:HB2	2.55	0.42
1:A:9:ALA:HB2	1:A:267:LYS:HB2	2.02	0.42
1:A:107:HIS:O	1:A:110:THR:O	2.38	0.42
1:B:208:GLU:OE1	1:B:210:LYS:NZ	2.41	0.42
1:B:102:ASP:HA	1:B:103:PRO:HD2	1.80	0.41
1:A:87:HIS:ND1	1:B:87:HIS:ND1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HD11	1:A:244:ASN:HD22	1.84	0.41
1:B:174:VAL:HG11	1:B:182:LEU:CD1	2.48	0.41
1:B:47:VAL:HG11	1:B:129:ALA:CB	2.50	0.41
1:A:278:LYS:HE3	4:B:478:HOH:O	2.20	0.41
1:B:107:HIS:H	1:B:107:HIS:CD2	2.39	0.41
1:A:133:GLN:CD	1:A:135:LYS:HE3	2.45	0.41
1:B:92:ASN:OD1	1:B:129:ALA:N	2.27	0.41
1:B:114:GLY:HA2	1:B:151:THR:HB	2.02	0.41
1:B:142:ILE:CD1	1:B:155:VAL:HG22	2.50	0.41
1:B:153:TRP:CZ3	1:B:205:PHE:HE2	2.39	0.41
1:B:219:ILE:HD12	1:B:219:ILE:H	1.86	0.41
1:B:282:ILE:N	4:B:477:HOH:O	2.54	0.41
1:A:34:LEU:HD12	1:A:34:LEU:O	2.21	0.41
1:A:144:ALA:CB	1:A:204:ALA:HB3	2.51	0.41
1:B:99:THR:HG22	1:B:222:THR:HG22	2.02	0.40
1:B:107:HIS:CD2	1:B:107:HIS:N	2.89	0.40
1:A:194:ILE:HB	1:A:195:PRO:HD3	2.03	0.40
1:B:77:LEU:HA	1:B:77:LEU:HD23	1.76	0.40
1:A:99:THR:CB	1:A:222:THR:HG22	2.46	0.40

There are no symmetry-related clashes.

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	280/286 (98%)	261 (93%)	18 (6%)	1 (0%)	30	43
1	B	280/286 (98%)	262 (94%)	17 (6%)	1 (0%)	30	43
All	All	560/572 (98%)	523 (93%)	35 (6%)	2 (0%)	30	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	ALA
1	B	195	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	244/247 (99%)	220 (90%)	24 (10%)	7	12
1	B	244/247 (99%)	220 (90%)	24 (10%)	7	12
All	All	488/494 (99%)	440 (90%)	48 (10%)	7	12

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	12	THR
1	A	13	LEU
1	A	24	LYS
1	A	27	SER
1	A	57	LEU
1	A	105	VAL
1	A	107	HIS
1	A	115	ASP
1	A	135	LYS
1	A	143	MET
1	A	164	LEU
1	A	176	LYS
1	A	182	LEU
1	A	186	ASN
1	A	193	LYS
1	A	202	GLN
1	A	222	THR
1	A	228	GLN
1	A	246	THR
1	A	247	LEU
1	A	255	LYS

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Mol	Chain	Res	Type
1	A	267	LYS
1	A	275	SER
1	B	13	LEU
1	B	21	LYS
1	B	26	VAL
1	B	34	LEU
1	B	38	LYS
1	B	39	GLU
1	B	59	ILE
1	B	64	THR
1	B	65	LEU
1	B	105	VAL
1	B	107	HIS
1	B	117	ASP
1	B	135	LYS
1	B	171	ILE
1	B	172	GLU
1	B	182	LEU
1	B	193	LYS
1	B	206	SER
1	B	212	LYS
1	B	220	LYS
1	B	227	LYS
1	B	247	LEU
1	B	249	ASP
1	B	274	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	30	HIS
1	A	40	ASN
1	A	107	HIS
1	A	133	GLN
1	A	202	GLN
1	B	11	ASN
1	B	40	ASN
1	B	54	ASN
1	B	107	HIS
1	B	133	GLN
1	B	169	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z > 2$
3	PO4	A	302	2	4,4,4	2.03	1 (25%)	6,6,6	1.35	0
3	PO4	A	301	2	4,4,4	1.42	1 (25%)	6,6,6	0.89	0
3	PO4	B	301	2	4,4,4	1.22	0	6,6,6	0.73	0
3	PO4	B	302	2	4,4,4	1.89	1 (25%)	6,6,6	1.22	1 (16%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	PO4	P-O1	3.97	1.59	1.50
3	B	302	PO4	P-O1	3.71	1.59	1.50
3	A	301	PO4	P-O3	2.30	1.61	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	PO4	O2-P-O1	-2.13	103.44	110.95

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
3	A	301	PO4	1	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](#)

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, 95th 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 ²)	Q<0.9
1	A	282/286 (98%)	-0.88	0 100 100	8, 25, 53, 83	0
1	B	282/286 (98%)	-0.77	0 100 100	8, 28, 61, 81	0
All	All	564/572 (98%)	-0.83	0 100 100	8, 26, 58, 83	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
2	MN	A	403	1/1	0.97	0.03	23,23,23,23	0
2	MN	B	404	1/1	0.97	0.03	23,23,23,23	0
2	MN	B	402	1/1	0.98	0.03	25,25,25,25	0
2	MN	B	403	1/1	0.98	0.02	27,27,27,27	0
2	MN	B	401	1/1	0.98	0.03	25,25,25,25	0
3	PO4	A	302	5/5	0.98	0.07	22,23,28,31	0
3	PO4	B	301	5/5	0.98	0.05	17,23,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	A	402	1/1	0.99	0.02	21,21,21,21	0
3	PO4	A	301	5/5	0.99	0.04	13,17,23,25	0
2	MN	A	401	1/1	0.99	0.02	15,15,15,15	0
2	MN	A	404	1/1	0.99	0.02	27,27,27,27	0
3	PO4	B	302	5/5	0.99	0.05	30,31,36,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.