



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:03 PM UTC

PDB ID : 2INU / pdb_00002inu
Title : Crystal structure of Inulin fructotransferase in the absence of substrate
Authors : Rhee, S.; Jung, W.S.
Deposited on : 2006-10-09
Resolution : 1.80 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

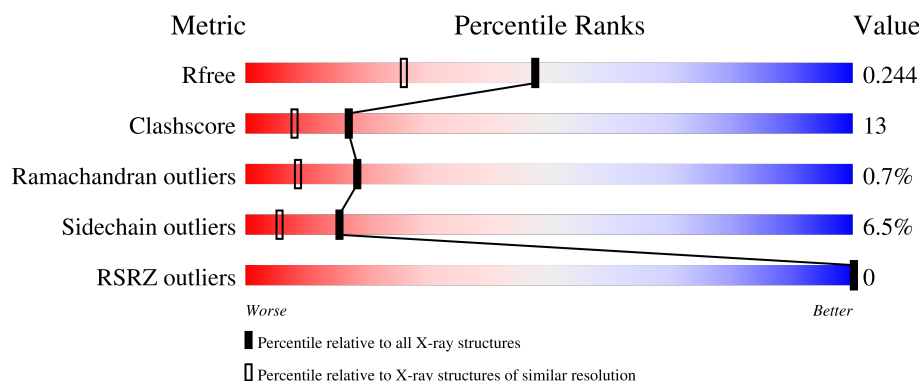
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	410	 65% 27% 5% 1% 2%
1	B	410	 63% 29% 5% 1% 2%
1	C	410	 66% 25% 5% 1% 2%

2 Entry composition [i](#)

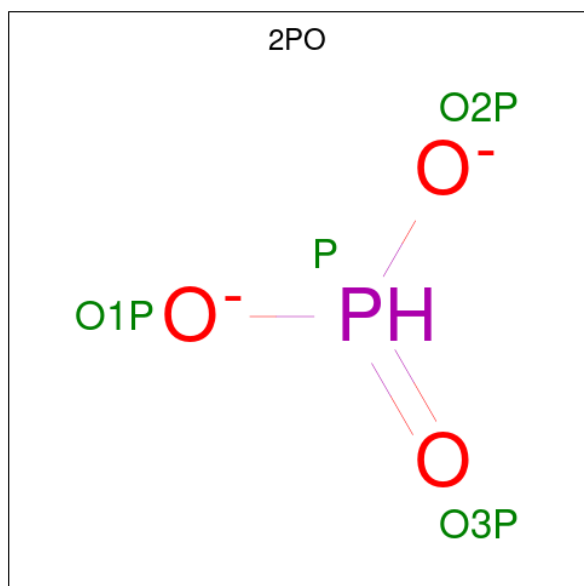
There are 3 unique types of molecules in this entry. The entry contains 9530 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Inulin fructotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			
1	B	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			
1	C	399	Total	C	N	O	S	Se	0	0	0
			2982	1859	535	578	6	4			

- Molecule 2 is PHOSPHONATE (CCD ID: 2PO) (formula: HO_3P).



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

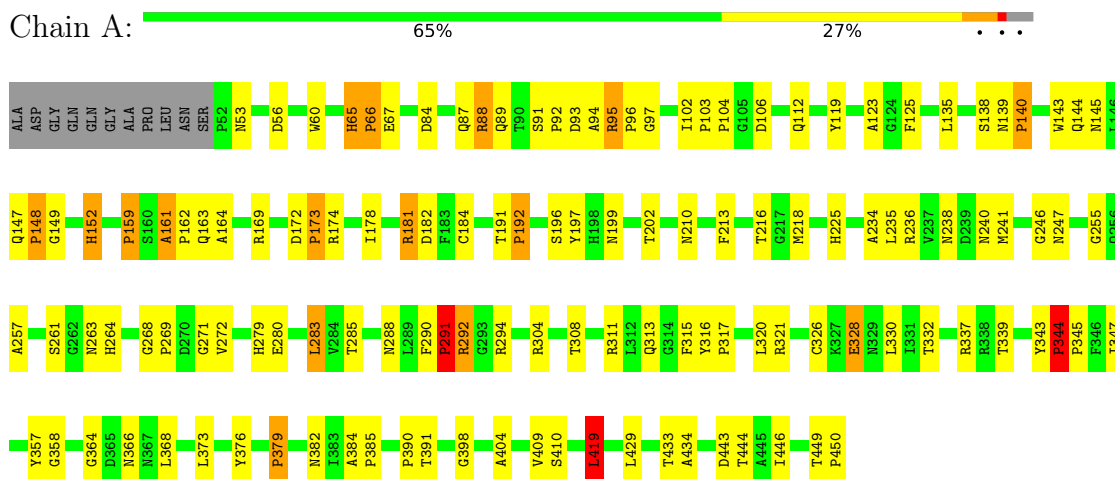
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	185	Total 185	O 185	0	0
3	B	195	Total 195	O 195	0	0
3	C	196	Total 196	O 196	0	0

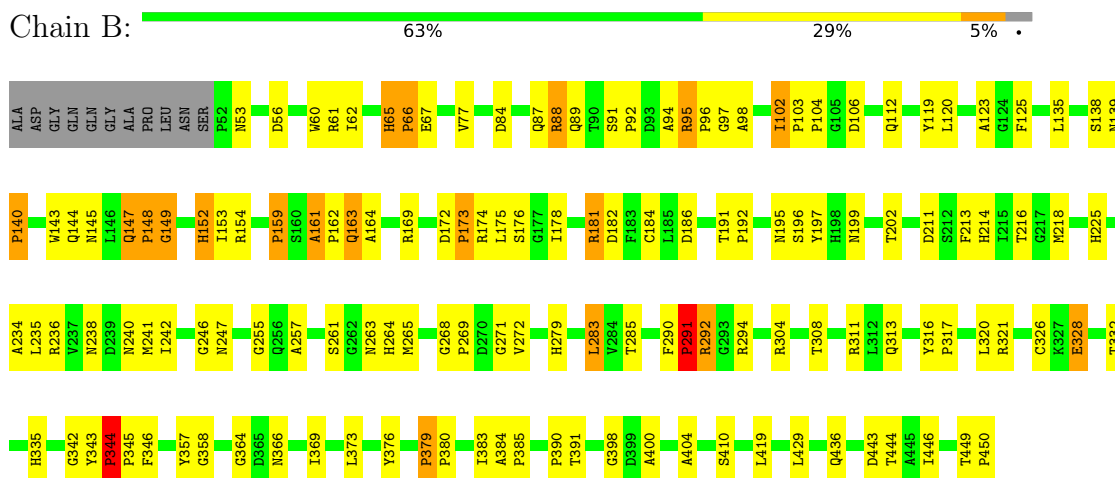
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

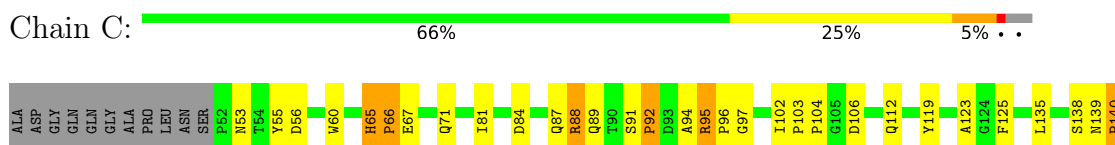
• Molecule 1: Inulin fructotransferase

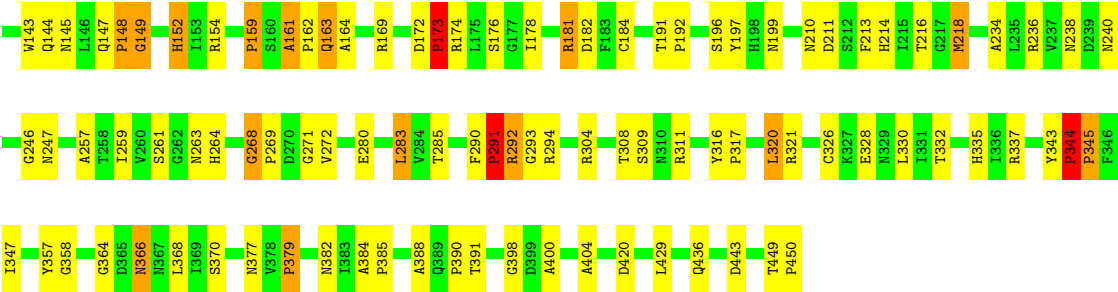


• Molecule 1: Inulin fructotransferase



• Molecule 1: Inulin fructotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.14Å 91.91Å 93.02Å 90.00° 124.75° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	74.1 (30.00-1.80) 98.4 (30.00-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.226 0.218 , 0.244	Depositor DCC
R_{free} test set	10149 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.003 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.011 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.012 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.018 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.018 for $-h+k-l, -l, -k$ 0.002 for $-h-k-l, l, k$ 0.019 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.003 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.489 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.489 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.013 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9530	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

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.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 2PO

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	0.61	7/3042 (0.2%)	1.50	46/4143 (1.1%)
1	B	0.59	6/3042 (0.2%)	1.50	51/4143 (1.2%)
1	C	0.59	6/3042 (0.2%)	1.76	52/4143 (1.3%)
All	All	0.60	19/9126 (0.2%)	1.59	149/12429 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	PRO	C-N	9.28	1.46	1.33
1	B	291	PRO	C-N	9.27	1.46	1.33
1	C	291	PRO	C-N	8.39	1.45	1.33
1	A	320	LEU	CB-CG	7.71	1.68	1.53
1	A	419	LEU	CG-CD2	-6.14	1.32	1.52
1	C	320	LEU	CG-CD1	-5.92	1.33	1.52
1	B	320	LEU	CB-CG	5.86	1.65	1.53
1	A	320	LEU	CG-CD1	-5.66	1.33	1.52
1	B	120	LEU	CG-CD1	5.35	1.70	1.52
1	A	240	ASN	CG-OD1	5.26	1.33	1.23
1	B	240	ASN	CG-OD1	5.25	1.33	1.23
1	C	292	ARG	C-N	-5.23	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	ARG	N-CA	5.22	1.56	1.46
1	B	292	ARG	N-CA	5.20	1.56	1.46
1	C	292	ARG	N-CA	5.19	1.56	1.46
1	C	240	ASN	CG-OD1	5.12	1.33	1.23
1	A	263	ASN	CG-OD1	5.12	1.33	1.23
1	B	263	ASN	CG-OD1	5.09	1.33	1.23
1	C	263	ASN	CG-OD1	5.04	1.33	1.23

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	172	ASP	CA-C-N	47.90	179.72	119.84
1	C	172	ASP	C-N-CA	47.90	179.72	119.84
1	B	291	PRO	O-C-N	-35.10	75.25	122.64
1	C	291	PRO	O-C-N	-34.63	75.89	122.64
1	A	291	PRO	O-C-N	-33.50	77.41	122.64
1	B	172	ASP	CA-C-N	21.84	179.42	127.00
1	B	172	ASP	C-N-CA	21.84	179.42	127.00
1	A	172	ASP	CA-C-N	21.35	178.23	127.00
1	A	172	ASP	C-N-CA	21.35	178.23	127.00
1	B	172	ASP	C-N-CD	-20.76	74.94	120.60
1	A	172	ASP	C-N-CD	-20.25	76.06	120.60
1	A	449	THR	N-CA-C	-12.68	90.65	109.42
1	B	449	THR	N-CA-C	-12.55	90.85	109.42
1	C	449	THR	N-CA-C	-12.50	90.92	109.42
1	C	172	ASP	C-N-CD	-12.19	75.03	125.00
1	A	95	ARG	CA-C-N	11.95	132.32	119.05
1	A	95	ARG	C-N-CA	11.95	132.32	119.05
1	C	95	ARG	CA-C-N	11.84	132.19	119.05
1	C	95	ARG	C-N-CA	11.84	132.19	119.05
1	B	95	ARG	CA-C-N	11.55	131.98	119.28
1	B	95	ARG	C-N-CA	11.55	131.98	119.28
1	C	147	GLN	N-CA-C	9.04	118.74	108.25
1	B	147	GLN	N-CA-C	8.92	118.60	108.25
1	A	147	GLN	N-CA-C	8.87	118.54	108.25
1	A	384	ALA	C-N-CD	-8.59	101.70	120.60
1	A	291	PRO	N-CA-C	8.52	130.02	112.47
1	B	384	ALA	C-N-CD	-8.48	101.95	120.60
1	C	384	ALA	C-N-CD	-8.47	101.96	120.60
1	B	291	PRO	N-CA-C	8.46	129.89	112.47
1	C	291	PRO	N-CA-C	8.44	129.86	112.47
1	B	294	ARG	N-CA-C	-8.31	102.59	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ARG	N-CA-C	-8.27	102.64	112.89
1	C	294	ARG	N-CA-C	-7.68	102.55	112.23
1	A	191	THR	C-N-CD	-7.53	104.05	120.60
1	C	191	THR	C-N-CD	-7.43	104.25	120.60
1	A	191	THR	CA-C-N	7.21	144.32	127.00
1	A	191	THR	C-N-CA	7.21	144.32	127.00
1	A	343	TYR	CA-C-N	7.20	127.80	120.38
1	A	343	TYR	C-N-CA	7.20	127.80	120.38
1	B	65	HIS	CA-C-N	7.20	127.52	119.32
1	B	65	HIS	C-N-CA	7.20	127.52	119.32
1	B	191	THR	C-N-CD	-7.16	104.86	120.60
1	A	65	HIS	CA-C-N	7.11	127.42	119.32
1	A	65	HIS	C-N-CA	7.11	127.42	119.32
1	C	181	ARG	N-CA-C	7.10	119.86	109.07
1	B	343	TYR	CA-C-N	7.08	127.67	120.38
1	B	343	TYR	C-N-CA	7.08	127.67	120.38
1	C	65	HIS	CA-C-N	7.04	127.34	119.32
1	C	65	HIS	C-N-CA	7.04	127.34	119.32
1	C	343	TYR	CA-C-N	6.99	127.58	120.38
1	C	343	TYR	C-N-CA	6.99	127.58	120.38
1	C	344	PRO	N-CA-C	6.85	119.06	110.70
1	A	344	PRO	N-CA-C	6.85	119.05	110.70
1	B	344	PRO	N-CA-C	6.83	119.04	110.70
1	A	181	ARG	N-CA-C	6.81	119.42	109.07
1	A	174	ARG	N-CA-C	-6.77	101.59	110.53
1	A	139	ASN	CA-C-N	6.70	126.39	119.82
1	A	139	ASN	C-N-CA	6.70	126.39	119.82
1	B	181	ARG	N-CA-C	6.65	119.18	109.07
1	C	88	ARG	N-CA-C	6.65	118.33	111.14
1	B	316	TYR	CA-C-N	6.63	126.61	119.78
1	B	316	TYR	C-N-CA	6.63	126.61	119.78
1	B	174	ARG	N-CA-C	-6.61	101.80	110.53
1	A	88	ARG	N-CA-C	6.60	118.27	111.14
1	C	139	ASN	CA-C-N	6.59	126.28	119.82
1	C	139	ASN	C-N-CA	6.59	126.28	119.82
1	C	191	THR	CA-C-N	6.54	142.70	127.00
1	C	191	THR	C-N-CA	6.54	142.70	127.00
1	B	139	ASN	CA-C-N	6.52	126.21	119.82
1	B	139	ASN	C-N-CA	6.52	126.21	119.82
1	C	316	TYR	CA-C-N	6.39	126.36	119.78
1	C	316	TYR	C-N-CA	6.39	126.36	119.78
1	C	174	ARG	N-CA-C	-6.36	101.53	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184	CYS	N-CA-C	6.29	119.15	108.90
1	A	184	CYS	N-CA-C	6.26	119.10	108.90
1	A	316	TYR	CA-C-N	6.23	126.20	119.78
1	A	316	TYR	C-N-CA	6.23	126.20	119.78
1	B	182	ASP	N-CA-C	6.12	119.86	111.54
1	B	191	THR	CA-C-N	6.01	141.42	127.00
1	B	191	THR	C-N-CA	6.01	141.42	127.00
1	B	184	CYS	N-CA-C	5.97	118.64	108.90
1	A	268	GLY	CA-C-N	5.94	126.09	119.32
1	A	268	GLY	C-N-CA	5.94	126.09	119.32
1	B	147	GLN	CA-C-N	5.89	125.84	119.78
1	B	147	GLN	C-N-CA	5.89	125.84	119.78
1	A	164	ALA	N-CA-C	-5.87	104.89	111.28
1	C	164	ALA	N-CA-C	-5.86	104.97	111.36
1	B	164	ALA	N-CA-C	-5.86	104.81	111.14
1	A	147	GLN	CA-C-N	5.85	125.80	119.78
1	A	147	GLN	C-N-CA	5.85	125.80	119.78
1	C	366	ASN	N-CA-C	5.84	119.61	111.90
1	B	366	ASN	N-CA-C	5.83	119.60	111.90
1	A	366	ASN	N-CA-C	5.78	119.53	111.90
1	C	268	GLY	CA-C-N	5.74	125.86	119.32
1	C	268	GLY	C-N-CA	5.74	125.86	119.32
1	B	268	GLY	CA-C-N	5.72	125.84	119.32
1	B	268	GLY	C-N-CA	5.72	125.84	119.32
1	A	182	ASP	N-CA-C	5.70	119.30	111.54
1	A	328	GLU	N-CA-C	5.69	119.24	111.39
1	A	56	ASP	N-CA-C	-5.68	99.16	108.41
1	C	102	ILE	CA-C-N	5.61	126.16	120.38
1	C	102	ILE	C-N-CA	5.61	126.16	120.38
1	B	218	MSE	N-CA-C	5.59	118.10	110.55
1	B	60	TRP	N-CA-C	5.59	117.41	108.41
1	B	102	ILE	CA-C-N	5.57	126.11	120.38
1	B	102	ILE	C-N-CA	5.57	126.11	120.38
1	C	60	TRP	N-CA-C	5.56	117.37	108.41
1	C	328	GLU	N-CA-C	5.56	119.10	111.54
1	C	56	ASP	N-CA-C	-5.53	99.39	108.41
1	C	147	GLN	CA-C-N	5.53	125.84	119.92
1	C	147	GLN	C-N-CA	5.53	125.84	119.92
1	C	182	ASP	N-CA-C	5.53	119.06	111.54
1	C	149	GLY	N-CA-C	5.50	118.85	111.20
1	B	328	GLU	N-CA-C	5.50	119.03	111.54
1	C	357	TYR	N-CA-C	-5.47	105.47	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	GLY	N-CA-C	5.47	118.80	111.20
1	B	56	ASP	N-CA-C	-5.45	99.53	108.41
1	A	60	TRP	N-CA-C	5.43	117.16	108.41
1	B	400	ALA	N-CA-C	5.42	119.48	112.86
1	C	152	HIS	N-CA-C	5.42	117.07	108.67
1	A	357	TYR	N-CA-C	-5.41	105.55	111.82
1	A	102	ILE	CA-C-N	5.38	125.92	120.38
1	A	102	ILE	C-N-CA	5.38	125.92	120.38
1	C	218	MSE	N-CA-C	5.38	117.47	110.53
1	B	88	ARG	N-CA-C	5.37	117.95	111.40
1	C	216	THR	N-CA-C	5.36	117.34	109.24
1	B	436	GLN	N-CA-C	-5.32	106.17	113.30
1	B	419	LEU	CD1-CG-CD2	-5.31	99.12	110.80
1	B	152	HIS	N-CA-C	5.29	116.86	108.67
1	C	163	GLN	N-CA-C	5.26	117.94	110.10
1	C	400	ALA	N-CA-C	5.23	119.62	113.23
1	A	152	HIS	N-CA-C	5.20	116.78	108.41
1	B	216	THR	N-CA-C	5.20	117.28	109.23
1	A	321	ARG	N-CA-C	5.15	117.29	108.90
1	C	173	PRO	CA-N-CD	-5.15	104.79	112.00
1	B	357	TYR	N-CA-C	-5.15	105.85	111.82
1	A	216	THR	N-CA-C	5.14	117.00	109.24
1	C	321	ARG	N-CA-C	5.12	117.24	108.90
1	C	388	ALA	N-CA-C	5.11	118.04	110.48
1	A	218	MSE	N-CA-C	5.10	117.43	110.55
1	B	163	GLN	N-CA-C	5.09	117.59	109.96
1	C	436	GLN	N-CA-C	-5.09	106.48	113.30
1	B	161	ALA	CA-C-N	5.08	126.19	119.84
1	B	161	ALA	C-N-CA	5.08	126.19	119.84
1	A	161	ALA	CA-C-N	5.08	126.18	119.84
1	A	161	ALA	C-N-CA	5.08	126.18	119.84
1	C	161	ALA	CA-C-N	5.07	126.18	119.84
1	C	161	ALA	C-N-CA	5.07	126.18	119.84
1	B	321	ARG	N-CA-C	5.05	117.30	108.76

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	PRO	Mainchain
1	B	291	PRO	Mainchain
1	C	291	PRO	Mainchain

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	2982	0	2905	90	0
1	B	2982	0	2905	92	0
1	C	2982	0	2905	87	0
2	A	4	0	1	0	0
2	B	4	0	1	0	0
3	A	185	0	0	2	0
3	B	195	0	0	2	0
3	C	196	0	0	1	0
All	All	9530	0	8717	224	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 13.

All (224) 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:B:283:LEU:HD22	1:B:285:THR:HG23	1.68	0.76
1:B:169:ARG:HH12	1:C:145:ASN:HD21	1.35	0.75
1:A:145:ASN:HD21	1:C:169:ARG:HH12	1.35	0.74
1:B:89:GLN:HE22	1:B:97:GLY:H	1.35	0.74
1:A:283:LEU:HD22	1:A:285:THR:HG23	1.68	0.74
1:C:95:ARG:N	1:C:96:PRO:HD3	2.03	0.74
1:B:95:ARG:N	1:B:96:PRO:HD3	2.02	0.73
1:A:89:GLN:HE22	1:A:97:GLY:H	1.37	0.72
1:A:236:ARG:HH21	1:B:264:HIS:HD2	1.37	0.72
1:C:138:SER:O	1:C:140:PRO:HD3	1.89	0.72
1:A:95:ARG:N	1:A:96:PRO:HD3	2.04	0.71
1:A:138:SER:O	1:A:140:PRO:HD3	1.93	0.68
1:A:169:ARG:HH12	1:B:145:ASN:HD21	1.41	0.68
1:A:91:SER:HB2	1:A:94:ALA:HB3	1.76	0.68
1:A:91:SER:O	1:A:95:ARG:HG3	1.94	0.68
1:B:138:SER:O	1:B:140:PRO:HD3	1.93	0.67
1:C:53:ASN:HD22	1:C:88:ARG:HH22	1.42	0.67
1:C:247:ASN:HD22	1:C:272:VAL:HG22	1.61	0.66
1:A:344:PRO:HB2	1:A:345:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LEU:HD22	1:C:285:THR:HG23	1.79	0.65
1:C:89:GLN:HE22	1:C:97:GLY:H	1.41	0.65
1:C:91:SER:O	1:C:95:ARG:HG3	1.97	0.64
1:B:344:PRO:HB2	1:B:345:PRO:HD3	1.80	0.63
1:A:283:LEU:HD22	1:A:285:THR:CG2	2.30	0.62
1:B:91:SER:O	1:B:95:ARG:HG3	2.00	0.61
1:C:91:SER:HB2	1:C:94:ALA:HB3	1.82	0.61
1:A:247:ASN:HD22	1:A:272:VAL:HG22	1.65	0.61
1:A:234:ALA:HB1	1:B:241:MSE:HE1	1.82	0.61
1:A:144:GLN:H	1:C:173:PRO:HD2	1.66	0.60
1:C:344:PRO:HB2	1:C:345:PRO:HD3	1.82	0.60
1:A:143:TRP:CE3	1:C:173:PRO:HG3	2.35	0.60
1:A:269:PRO:HD3	1:A:292:ARG:HG3	1.82	0.60
1:C:337:ARG:HH22	1:C:377:ASN:HB3	1.66	0.60
1:B:247:ASN:HD22	1:B:272:VAL:HG22	1.66	0.60
1:B:89:GLN:O	1:B:95:ARG:HD3	2.02	0.60
1:B:269:PRO:HD3	1:B:292:ARG:HG3	1.84	0.60
1:C:89:GLN:HB3	1:C:95:ARG:HG2	1.84	0.60
1:A:241:MSE:HE1	1:C:234:ALA:HB1	1.84	0.59
1:B:53:ASN:HD22	1:B:88:ARG:HH22	1.49	0.59
1:B:283:LEU:HD22	1:B:285:THR:CG2	2.31	0.59
1:B:173:PRO:HG3	1:C:143:TRP:CE3	2.38	0.59
1:C:269:PRO:HD3	1:C:292:ARG:HG3	1.85	0.59
1:A:89:GLN:O	1:A:95:ARG:HD3	2.03	0.58
1:A:236:ARG:HD3	3:B:1171:HOH:O	2.04	0.58
1:C:89:GLN:O	1:C:95:ARG:HD3	2.03	0.58
1:B:159:PRO:O	1:B:162:PRO:HD3	2.03	0.58
1:B:84:ASP:O	1:B:87:GLN:HB3	2.04	0.57
1:B:358:GLY:HA2	1:B:391:THR:O	2.04	0.57
1:A:53:ASN:HD22	1:A:88:ARG:HH22	1.52	0.57
1:A:94:ALA:C	1:A:96:PRO:HD3	2.30	0.57
1:A:173:PRO:HG3	1:B:143:TRP:CE3	2.40	0.56
1:A:311:ARG:HB2	1:C:283:LEU:HG	1.87	0.56
1:B:290:PHE:HB2	1:B:291:PRO:HD2	1.87	0.56
1:A:264:HIS:HD2	1:C:236:ARG:HH21	1.52	0.55
1:A:159:PRO:O	1:A:162:PRO:HD3	2.06	0.55
1:B:94:ALA:C	1:B:96:PRO:HD3	2.30	0.55
1:B:380:PRO:HA	1:B:383:ILE:HD12	1.89	0.55
1:A:84:ASP:O	1:A:87:GLN:HB3	2.07	0.55
1:A:106:ASP:CG	1:C:96:PRO:HG3	2.31	0.55
1:C:94:ALA:C	1:C:96:PRO:HD3	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:GLY:O	1:B:398:GLY:HA3	2.07	0.54
1:C:84:ASP:O	1:C:87:GLN:HB3	2.08	0.54
1:A:419:LEU:N	1:A:419:LEU:HD22	2.23	0.54
1:C:290:PHE:HB2	1:C:291:PRO:HD2	1.89	0.54
1:A:290:PHE:HB2	1:A:291:PRO:HD2	1.89	0.53
1:C:159:PRO:O	1:C:162:PRO:HD3	2.08	0.53
1:A:358:GLY:HA2	1:A:391:THR:O	2.08	0.53
1:C:71:GLN:HG3	3:C:497:HOH:O	2.08	0.53
1:C:358:GLY:HA2	1:C:391:THR:O	2.08	0.53
1:A:433:THR:HG22	1:A:434:ALA:N	2.24	0.53
1:C:283:LEU:HD22	1:C:285:THR:CG2	2.38	0.53
1:C:326:CYS:O	1:C:364:GLY:HA3	2.08	0.53
1:C:364:GLY:O	1:C:398:GLY:HA3	2.09	0.53
1:A:173:PRO:HD2	1:B:144:GLN:H	1.74	0.52
1:A:149:GLY:HA3	1:C:119:TYR:CD2	2.43	0.52
1:A:96:PRO:HG3	1:B:106:ASP:CG	2.34	0.52
1:A:148:PRO:HB2	1:A:152:HIS:CE1	2.44	0.52
1:B:96:PRO:HG3	1:C:106:ASP:CG	2.35	0.52
1:A:135:LEU:HD12	1:A:140:PRO:HG3	1.92	0.52
1:B:89:GLN:HB3	1:B:95:ARG:HG2	1.92	0.52
1:B:328:GLU:O	1:C:335:HIS:HE1	1.93	0.52
1:A:123:ALA:HA	1:A:181:ARG:O	2.10	0.51
1:B:326:CYS:O	1:B:364:GLY:HA3	2.10	0.51
1:B:53:ASN:ND2	1:B:88:ARG:HH22	2.08	0.51
1:C:246:GLY:O	1:C:271:GLY:HA3	2.11	0.51
1:C:337:ARG:HH22	1:C:377:ASN:CB	2.24	0.51
1:C:112:GLN:HG3	1:C:163:GLN:O	2.11	0.51
1:A:65:HIS:N	1:A:66:PRO:HD3	2.25	0.51
1:C:65:HIS:N	1:C:66:PRO:HD3	2.27	0.50
1:A:178:ILE:HD12	1:A:213:PHE:CZ	2.46	0.50
1:A:326:CYS:O	1:A:364:GLY:HA3	2.11	0.50
1:A:104:PRO:HB2	1:C:53:ASN:HB2	1.93	0.50
1:A:238:ASN:HA	1:A:261:SER:O	2.12	0.49
1:A:328:GLU:O	1:B:335:HIS:HE1	1.95	0.49
1:B:91:SER:HB3	1:B:94:ALA:HB3	1.93	0.49
1:A:169:ARG:HH22	1:B:145:ASN:HD22	1.60	0.49
1:C:238:ASN:HA	1:C:261:SER:O	2.12	0.49
3:A:1167:HOH:O	1:C:236:ARG:HD3	2.12	0.49
1:A:145:ASN:H	1:C:173:PRO:HG2	1.77	0.49
1:A:135:LEU:CD1	1:A:140:PRO:HG3	2.42	0.49
1:A:288:ASN:HB2	1:C:259:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LEU:HD12	1:C:140:PRO:HG3	1.95	0.49
1:B:178:ILE:HD12	1:B:213:PHE:CZ	2.47	0.49
1:C:154:ARG:HH11	1:C:154:ARG:HG2	1.77	0.49
1:A:161:ALA:N	1:A:162:PRO:HD3	2.28	0.49
1:A:119:TYR:CD2	1:B:149:GLY:HA3	2.47	0.48
1:C:178:ILE:HD12	1:C:213:PHE:CZ	2.48	0.48
1:B:119:TYR:CD2	1:C:149:GLY:HA3	2.49	0.48
1:B:238:ASN:HA	1:B:261:SER:O	2.14	0.48
1:C:123:ALA:HA	1:C:181:ARG:O	2.14	0.48
1:A:246:GLY:O	1:A:271:GLY:HA3	2.14	0.48
1:B:236:ARG:NH2	1:C:264:HIS:HD2	2.12	0.48
1:A:53:ASN:ND2	1:A:88:ARG:HH22	2.11	0.48
1:B:65:HIS:N	1:B:66:PRO:HD3	2.29	0.48
1:A:364:GLY:O	1:A:398:GLY:HA3	2.14	0.47
1:B:135:LEU:CD1	1:B:140:PRO:HG3	2.44	0.47
1:C:95:ARG:N	1:C:96:PRO:CD	2.73	0.47
1:A:112:GLN:HG3	1:A:163:GLN:O	2.14	0.47
1:A:53:ASN:CB	1:B:104:PRO:HB2	2.45	0.47
1:A:89:GLN:HB3	1:A:95:ARG:HG2	1.94	0.47
1:C:148:PRO:HB2	1:C:152:HIS:CE1	2.49	0.47
1:B:53:ASN:CB	1:C:104:PRO:HB2	2.44	0.47
1:B:112:GLN:HG3	1:B:163:GLN:O	2.14	0.47
1:A:292:ARG:HA	3:A:1017:HOH:O	2.14	0.47
1:A:236:ARG:HH21	1:B:264:HIS:CD2	2.25	0.47
1:A:283:LEU:HG	1:B:311:ARG:HB2	1.97	0.47
1:C:404:ALA:HA	1:C:429:LEU:O	2.14	0.47
1:A:311:ARG:HD3	1:A:311:ARG:C	2.39	0.47
1:C:161:ALA:N	1:C:162:PRO:HD3	2.31	0.46
1:B:234:ALA:HA	1:B:257:ALA:O	2.16	0.46
1:C:210:ASN:HB2	1:C:213:PHE:CE1	2.50	0.46
1:A:404:ALA:HA	1:A:429:LEU:O	2.16	0.46
1:B:123:ALA:HA	1:B:181:ARG:O	2.15	0.46
1:A:145:ASN:ND2	1:C:169:ARG:HH12	2.10	0.46
1:A:95:ARG:N	1:A:96:PRO:CD	2.75	0.46
1:A:138:SER:C	1:A:140:PRO:HD3	2.41	0.46
1:B:173:PRO:HD2	1:C:144:GLN:H	1.79	0.46
1:A:53:ASN:HD21	1:A:88:ARG:HH12	1.64	0.45
1:A:344:PRO:HA	1:A:347:ILE:HD12	1.96	0.45
1:B:53:ASN:HB2	1:C:104:PRO:HB2	1.97	0.45
1:B:104:PRO:HD3	1:B:125:PHE:CD1	2.52	0.45
1:B:195:ASN:HB3	1:B:346:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:OD1	1:A:152:HIS:HD2	2.00	0.45
1:B:246:GLY:O	1:B:271:GLY:HA3	2.17	0.45
1:B:283:LEU:HG	1:C:311:ARG:HB2	1.98	0.45
1:C:308:THR:HG22	1:C:309:SER:N	2.32	0.45
1:C:379:PRO:HB2	1:C:382:ASN:ND2	2.32	0.45
1:B:161:ALA:N	1:B:162:PRO:HD3	2.31	0.44
1:C:214:HIS:CE1	1:C:236:ARG:HD2	2.51	0.44
1:A:104:PRO:HB2	1:C:53:ASN:CB	2.46	0.44
1:B:61:ARG:HD2	3:B:1156:HOH:O	2.17	0.44
1:A:53:ASN:HB2	1:B:104:PRO:HB2	1.99	0.44
1:B:404:ALA:HA	1:B:429:LEU:O	2.17	0.44
1:C:53:ASN:ND2	1:C:88:ARG:HH22	2.09	0.44
1:B:242:ILE:O	1:B:265:MSE:HA	2.18	0.44
1:B:342:GLY:O	1:B:344:PRO:HD3	2.18	0.44
1:C:135:LEU:CD1	1:C:140:PRO:HG3	2.48	0.44
1:A:330:LEU:HD13	1:A:368:LEU:HD23	1.99	0.44
1:B:148:PRO:HB2	1:B:152:HIS:CE1	2.53	0.44
1:B:291:PRO:HD3	1:B:313:GLN:HB3	2.00	0.44
1:A:255:GLY:HA3	1:A:279:HIS:CE1	2.52	0.43
1:B:196:SER:O	1:B:197:TYR:HB2	2.18	0.43
1:C:196:SER:O	1:C:197:TYR:HB2	2.17	0.43
1:C:344:PRO:HA	1:C:347:ILE:HD12	2.00	0.43
1:A:169:ARG:HH22	1:B:145:ASN:ND2	2.14	0.43
1:A:145:ASN:HD22	1:C:169:ARG:HH22	1.67	0.43
1:C:55:TYR:CE2	1:C:81:ILE:HG23	2.54	0.43
1:C:218:MSE:HE3	1:C:218:MSE:HB3	1.88	0.43
1:B:135:LEU:HD12	1:B:140:PRO:HG3	2.00	0.43
1:B:376:TYR:O	1:B:410:SER:HA	2.19	0.43
1:C:104:PRO:HD3	1:C:125:PHE:CD1	2.54	0.43
1:A:202:THR:HA	1:A:225:HIS:O	2.18	0.42
1:C:311:ARG:HD3	1:C:311:ARG:C	2.44	0.42
1:B:106:ASP:OD1	1:B:152:HIS:HD2	2.01	0.42
1:C:53:ASN:HD21	1:C:88:ARG:HH12	1.67	0.42
1:A:308:THR:HA	1:A:332:THR:O	2.20	0.42
1:B:102:ILE:HD13	1:B:153:ILE:HD11	2.00	0.42
1:B:202:THR:HA	1:B:225:HIS:O	2.20	0.42
1:A:444:THR:HG22	1:A:446:ILE:HG13	2.01	0.42
1:B:53:ASN:O	1:B:98:ALA:HB1	2.20	0.42
1:A:93:ASP:CG	1:B:147:GLN:HE21	2.28	0.42
1:C:138:SER:C	1:C:140:PRO:HD3	2.43	0.42
1:B:152:HIS:HE1	1:B:186:ASP:OD2	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:GLU:O	1:C:67:GLU:HG3	2.20	0.42
1:C:370:SER:HA	1:C:404:ALA:O	2.19	0.41
1:B:214:HIS:HE1	1:B:238:ASN:OD1	2.03	0.41
1:B:373:LEU:C	1:B:373:LEU:HD23	2.44	0.41
1:A:376:TYR:O	1:A:410:SER:HA	2.21	0.41
1:B:169:ARG:HB2	1:B:175:LEU:HD11	2.03	0.41
1:B:444:THR:HG22	1:B:446:ILE:HG13	2.02	0.41
1:A:210:ASN:HB2	1:A:213:PHE:CE1	2.56	0.41
1:A:235:LEU:HG	1:A:236:ARG:N	2.36	0.41
1:A:315:PHE:HA	1:A:339:THR:O	2.20	0.41
1:A:373:LEU:C	1:A:373:LEU:HD23	2.45	0.41
1:B:255:GLY:HA3	1:B:279:HIS:CE1	2.55	0.41
1:A:196:SER:O	1:A:197:TYR:HB2	2.21	0.41
1:B:235:LEU:HD12	1:B:236:ARG:H	1.85	0.41
1:A:291:PRO:HD3	1:A:313:GLN:HB3	2.03	0.41
1:B:291:PRO:HD3	1:B:313:GLN:O	2.21	0.41
1:C:154:ARG:HG2	1:C:154:ARG:NH1	2.36	0.41
1:A:104:PRO:HD3	1:A:125:PHE:CD1	2.55	0.41
1:B:154:ARG:HG2	1:B:154:ARG:HH11	1.86	0.41
1:B:290:PHE:HB2	1:B:291:PRO:CD	2.50	0.41
1:B:311:ARG:HD3	1:B:311:ARG:C	2.46	0.41
1:B:379:PRO:O	1:B:380:PRO:C	2.64	0.41
1:C:176:SER:HA	1:C:211:ASP:O	2.20	0.41
1:C:234:ALA:HA	1:C:257:ALA:O	2.21	0.41
1:A:379:PRO:HB2	1:A:382:ASN:ND2	2.36	0.41
1:C:92:PRO:HG3	1:C:95:ARG:NH2	2.36	0.41
1:C:268:GLY:O	1:C:293:GLY:HA2	2.21	0.40
1:A:285:THR:HA	1:A:308:THR:O	2.22	0.40
1:C:330:LEU:HD13	1:C:368:LEU:HD23	2.03	0.40
1:B:62:ILE:HD11	1:B:77:VAL:HA	2.03	0.40
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.91	0.40
1:B:257:ALA:O	1:C:264:HIS:HE1	2.05	0.40
1:B:308:THR:HA	1:B:332:THR:O	2.22	0.40
1:C:308:THR:HA	1:C:332:THR:O	2.21	0.40
1:A:173:PRO:HG2	1:B:145:ASN:H	1.85	0.40
1:A:257:ALA:O	1:B:264:HIS:HE1	2.05	0.40
1:B:173:PRO:HG2	1:C:145:ASN:H	1.85	0.40
1:B:176:SER:HA	1:B:211:ASP:O	2.22	0.40
1:A:145:ASN:ND2	1:C:169:ARG:HH22	2.18	0.40
1:A:409:VAL:HG21	1:C:366:ASN:HB3	2.03	0.40
1:B:369:ILE:HD12	1:B:369:ILE:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	397/410 (97%)	372 (94%)	22 (6%)	3 (1%)	16	6
1	B	397/410 (97%)	372 (94%)	23 (6%)	2 (0%)	24	14
1	C	397/410 (97%)	370 (93%)	24 (6%)	3 (1%)	16	6
All	All	1191/1230 (97%)	1114 (94%)	69 (6%)	8 (1%)	18	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	173	PRO
1	A	199	ASN
1	B	199	ASN
1	C	199	ASN
1	B	291	PRO
1	A	291	PRO
1	C	291	PRO
1	A	192	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	322/325 (99%)	300 (93%)	22 (7%)	14	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	322/325 (99%)	303 (94%)	19 (6%)	18	7
1	C	322/325 (99%)	300 (93%)	22 (7%)	14	5
All	All	966/975 (99%)	903 (94%)	63 (6%)	15	5

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	A	67	GLU
1	A	92	PRO
1	A	103	PRO
1	A	140	PRO
1	A	148	PRO
1	A	159	PRO
1	A	173	PRO
1	A	192	PRO
1	A	280	GLU
1	A	283	LEU
1	A	291	PRO
1	A	304	ARG
1	A	317	PRO
1	A	337	ARG
1	A	344	PRO
1	A	379	PRO
1	A	385	PRO
1	A	390	PRO
1	A	419	LEU
1	A	443	ASP
1	A	450	PRO
1	B	66	PRO
1	B	67	GLU
1	B	92	PRO
1	B	103	PRO
1	B	140	PRO
1	B	148	PRO
1	B	159	PRO
1	B	173	PRO
1	B	192	PRO
1	B	283	LEU
1	B	291	PRO
1	B	304	ARG

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Mol	Chain	Res	Type
1	B	317	PRO
1	B	344	PRO
1	B	379	PRO
1	B	385	PRO
1	B	390	PRO
1	B	443	ASP
1	B	450	PRO
1	C	66	PRO
1	C	92	PRO
1	C	103	PRO
1	C	140	PRO
1	C	148	PRO
1	C	159	PRO
1	C	173	PRO
1	C	192	PRO
1	C	280	GLU
1	C	283	LEU
1	C	291	PRO
1	C	304	ARG
1	C	317	PRO
1	C	320	LEU
1	C	344	PRO
1	C	345	PRO
1	C	379	PRO
1	C	385	PRO
1	C	390	PRO
1	C	420	ASP
1	C	443	ASP
1	C	450	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	89	GLN
1	A	137	ASN
1	A	145	ASN
1	A	152	HIS
1	A	195	ASN
1	A	214	HIS
1	A	247	ASN
1	A	264	HIS

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Mol	Chain	Res	Type
1	A	313	GLN
1	A	324	ASN
1	A	389	GLN
1	A	392	GLN
1	A	425	HIS
1	B	53	ASN
1	B	89	GLN
1	B	137	ASN
1	B	145	ASN
1	B	152	HIS
1	B	195	ASN
1	B	214	HIS
1	B	238	ASN
1	B	247	ASN
1	B	264	HIS
1	B	313	GLN
1	B	324	ASN
1	B	335	HIS
1	B	416	HIS
1	B	425	HIS
1	C	53	ASN
1	C	89	GLN
1	C	137	ASN
1	C	145	ASN
1	C	152	HIS
1	C	195	ASN
1	C	247	ASN
1	C	256	GLN
1	C	264	HIS
1	C	313	GLN
1	C	324	ASN
1	C	335	HIS
1	C	377	ASN
1	C	416	HIS
1	C	425	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2PO	A	1002	-	0,3,3	-	-	0,3,3	-	-
2	2PO	B	1001	-	0,3,3	-	-	0,3,3	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	395/410 (96%)	-1.48	0 100 100	7, 13, 25, 32	0
1	B	395/410 (96%)	-1.48	0 100 100	7, 13, 25, 31	0
1	C	395/410 (96%)	-1.48	0 100 100	6, 13, 24, 31	0
All	All	1185/1230 (96%)	-1.48	0 100 100	6, 13, 25, 32	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	2PO	A	1002	4/4	0.96	0.05	56,56,56,56	0
2	2PO	B	1001	4/4	0.99	0.06	57,58,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.