



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:23 PM UTC

PDB ID : 1CYG / pdb_00001cyg
Title : CYCLODEXTRIN GLUCANOTRANSFERASE (E.C.2.4.1.19) (CGTASE)
Authors : Kubota, M.; Matsuura, Y.; Sakai, S.; Katsube, Y.
Deposited on : 1993-02-03
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

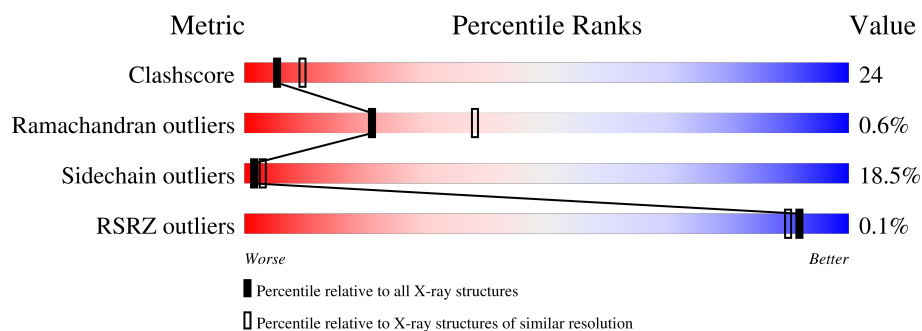
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

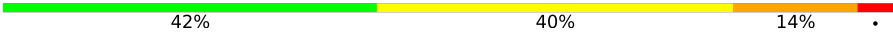
The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	680	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5551 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 CYCLODEXTRIN GLUCANOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	0	0	0
			5318	3347	905	1044	22			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

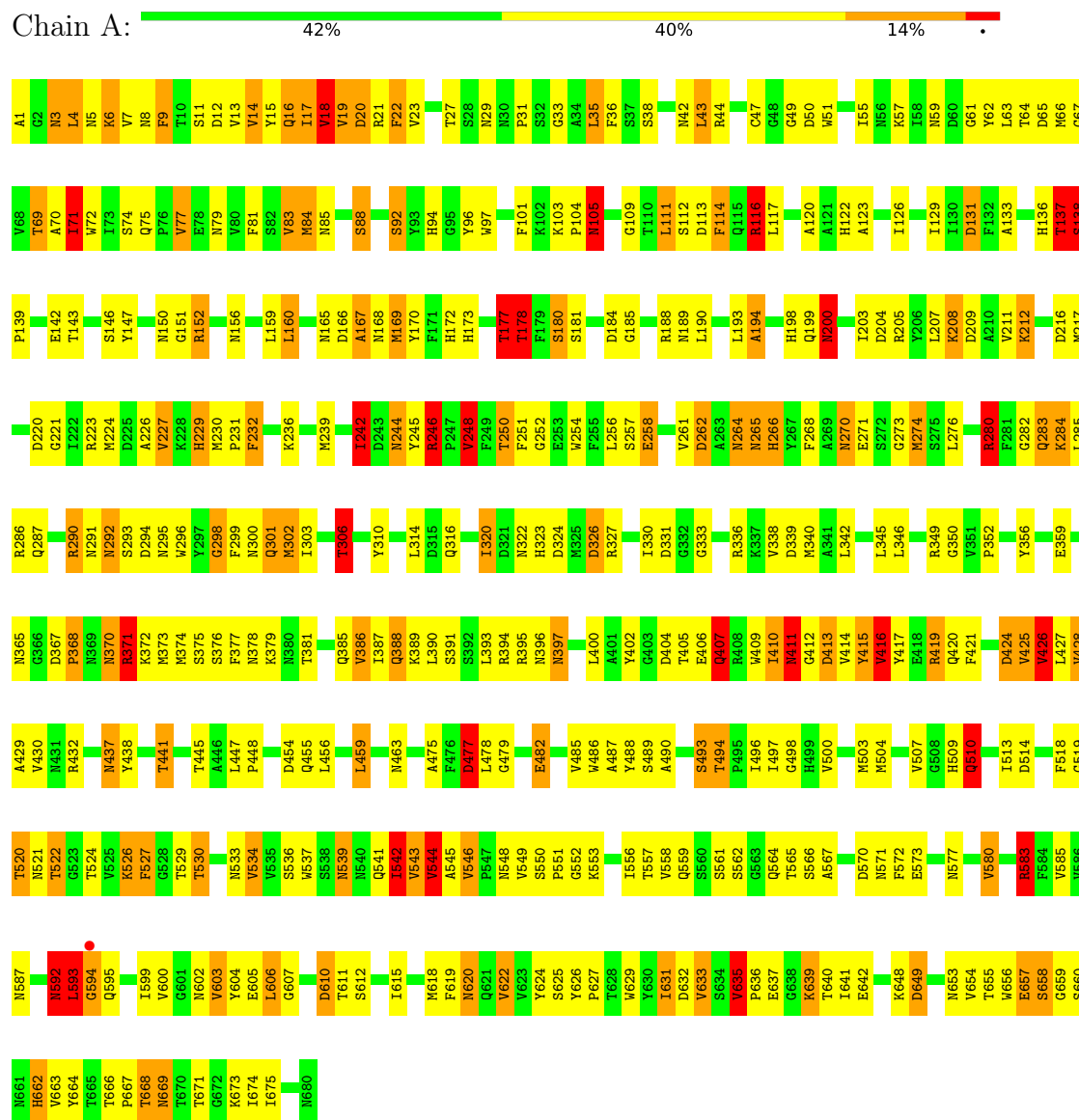
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	231	Total	O	0	0
			231	231		

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: CYCLODEXTRIN GLUCANOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.50Å 88.00Å 78.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.50 5.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.50) 85.3 (5.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.02Å)	Xtriage
Refinement program	PROFFT, PROLSQ	Depositor
R, R_{free}	0.154 , (Not available) 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	9.1	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.53 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5551	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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

5.1 Standard geometry

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

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	1.21	3/5447 (0.1%)	2.10	208/7411 (2.8%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	603	VAL	N-CA	6.18	1.53	1.46
1	A	17	ILE	CA-CB	5.26	1.60	1.54
1	A	530	THR	CA-CB	5.02	1.60	1.53

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ARG	CD-NE-CZ	20.88	153.63	124.40
1	A	416	VAL	CB-CA-C	12.64	125.77	110.73
1	A	229	HIS	CA-CB-CG	-10.70	103.10	113.80
1	A	411	ASN	CA-CB-CG	10.58	123.18	112.60
1	A	152	ARG	CD-NE-CZ	10.38	138.93	124.40
1	A	216	ASP	CA-CB-CG	9.44	122.03	112.60
1	A	477	ASP	CA-CB-CG	-9.33	103.27	112.60
1	A	280	ARG	O-C-N	9.33	131.68	122.07
1	A	230	MET	CB-CA-C	9.28	122.81	108.61
1	A	136	HIS	CA-CB-CG	-9.17	104.63	113.80
1	A	410	ILE	CA-C-N	8.90	137.77	122.82
1	A	410	ILE	C-N-CA	8.90	137.77	122.82
1	A	178	THR	N-CA-CB	-8.84	99.31	110.98
1	A	659	GLY	O-C-N	-8.68	116.54	123.14
1	A	327	ARG	CD-NE-CZ	8.59	136.43	124.40
1	A	412	GLY	N-CA-C	-8.53	103.84	114.16
1	A	189	ASN	CA-CB-CG	8.42	121.02	112.60
1	A	583	ARG	CD-NE-CZ	8.26	135.97	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	603	VAL	CB-CA-C	8.23	122.75	110.90
1	A	635	VAL	N-CA-CB	-8.22	99.70	111.21
1	A	657	GLU	N-CA-C	-8.09	99.09	110.50
1	A	549	VAL	O-C-N	8.07	130.20	122.69
1	A	105	ASN	O-C-N	8.06	127.76	121.23
1	A	18	VAL	CB-CA-C	7.61	121.89	112.45
1	A	463	ASN	OD1-CG-ND2	7.48	130.08	122.60
1	A	570	ASP	N-CA-C	7.43	122.13	110.32
1	A	527	PHE	CA-CB-CG	7.30	121.10	113.80
1	A	65	ASP	CA-CB-CG	-7.21	105.39	112.60
1	A	388	GLN	CA-CB-CG	7.19	128.49	114.10
1	A	211	VAL	CB-CA-C	7.14	121.39	112.04
1	A	160	LEU	CB-CA-C	7.12	121.26	110.08
1	A	160	LEU	N-CA-C	-7.09	103.50	112.93
1	A	264	ASN	O-C-N	7.09	130.23	122.15
1	A	333	GLY	CA-C-N	7.05	131.05	121.74
1	A	333	GLY	C-N-CA	7.05	131.05	121.74
1	A	4	LEU	CB-CA-C	7.05	122.51	109.54
1	A	658	SER	CA-C-O	-7.04	110.44	120.51
1	A	322	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	320	ILE	N-CA-CB	6.98	119.89	112.21
1	A	168	ASN	CA-CB-CG	6.93	119.53	112.60
1	A	567	ALA	N-CA-C	-6.92	101.40	110.53
1	A	61	GLY	N-CA-C	6.91	124.20	115.21
1	A	276	LEU	N-CA-CB	-6.91	98.67	111.52
1	A	16	GLN	CA-C-O	6.84	128.09	120.43
1	A	378	ASN	CA-CB-CG	6.83	119.43	112.60
1	A	320	ILE	O-C-N	6.78	129.10	122.25
1	A	526	LYS	CA-C-O	6.73	128.40	120.66
1	A	521	ASN	CB-CA-C	6.65	120.67	109.84
1	A	190	LEU	CB-CA-C	6.63	121.84	110.77
1	A	413	ASP	N-CA-C	6.60	121.37	113.12
1	A	320	ILE	N-CA-C	-6.55	106.29	113.43
1	A	276	LEU	N-CA-C	6.54	119.25	108.99
1	A	306	THR	CA-CB-CG2	6.51	121.57	110.50
1	A	137	THR	CA-C-N	6.50	131.43	122.07
1	A	137	THR	C-N-CA	6.50	131.43	122.07
1	A	327	ARG	NE-CZ-NH1	6.50	128.00	121.50
1	A	242	ILE	N-CA-CB	6.43	120.23	110.58
1	A	572	PHE	N-CA-CB	6.42	119.42	109.85
1	A	92	SER	CA-C-N	6.40	129.18	120.54
1	A	92	SER	C-N-CA	6.40	129.18	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	MET	CA-C-N	6.39	132.32	121.14
1	A	84	MET	C-N-CA	6.39	132.32	121.14
1	A	152	ARG	CA-C-O	6.39	128.18	121.15
1	A	71	ILE	N-CA-CB	-6.38	102.57	111.25
1	A	426	VAL	O-C-N	6.37	129.81	123.18
1	A	605	GLU	CB-CG-CD	6.37	123.43	112.60
1	A	610	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	594	GLY	N-CA-C	-6.28	107.10	115.32
1	A	246	ARG	CD-NE-CZ	6.27	133.17	124.40
1	A	116	ARG	CD-NE-CZ	-6.26	115.63	124.40
1	A	282	GLY	CA-C-N	6.24	128.93	120.38
1	A	282	GLY	C-N-CA	6.24	128.93	120.38
1	A	114	PHE	CA-CB-CG	-6.24	107.56	113.80
1	A	551	PRO	CB-CA-C	6.22	119.19	111.23
1	A	631	ILE	O-C-N	6.19	129.13	123.19
1	A	280	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	A	232	PHE	N-CA-CB	6.12	120.83	110.49
1	A	656	TRP	O-C-N	6.11	129.81	122.85
1	A	640	THR	CB-CA-C	6.07	120.36	110.22
1	A	370	ASN	CA-CB-CG	6.05	118.65	112.60
1	A	494	THR	O-C-N	6.05	128.54	121.10
1	A	386	VAL	N-CA-CB	6.04	118.76	110.54
1	A	539	ASN	OD1-CG-ND2	6.04	128.64	122.60
1	A	390	LEU	CB-CA-C	6.03	122.25	110.67
1	A	577	ASN	N-CA-CB	-6.02	100.31	110.49
1	A	587	ASN	OD1-CG-ND2	6.02	128.62	122.60
1	A	326	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	88	SER	N-CA-C	5.98	117.87	111.36
1	A	71	ILE	CB-CA-C	5.97	119.72	110.83
1	A	571	ASN	CA-CB-CG	5.96	118.56	112.60
1	A	189	ASN	O-C-N	5.96	130.26	122.93
1	A	246	ARG	NE-CZ-NH1	5.95	127.45	121.50
1	A	172	HIS	CA-CB-CG	5.93	119.73	113.80
1	A	181	SER	O-C-N	5.93	129.49	123.26
1	A	407	GLN	CA-CB-CG	5.93	125.97	114.10
1	A	9	PHE	CA-CB-CG	5.92	119.72	113.80
1	A	120	ALA	N-CA-C	-5.92	104.91	111.71
1	A	198	HIS	CA-CB-CG	-5.90	107.90	113.80
1	A	18	VAL	CA-C-N	5.89	132.57	121.97
1	A	18	VAL	C-N-CA	5.89	132.57	121.97
1	A	270	ASN	N-CA-C	5.89	118.65	111.82
1	A	415	TYR	CA-C-N	-5.88	114.99	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	TYR	C-N-CA	-5.88	114.99	123.11
1	A	463	ASN	N-CA-CB	-5.84	101.55	110.49
1	A	120	ALA	O-C-N	5.80	129.00	122.22
1	A	580	VAL	CA-C-O	-5.79	115.90	121.63
1	A	327	ARG	CA-CB-CG	5.78	125.65	114.10
1	A	248	VAL	N-CA-CB	-5.77	101.99	111.45
1	A	397	ASN	CB-CA-C	5.71	116.65	110.08
1	A	627	PRO	N-CD-CG	-5.71	96.95	103.80
1	A	424	ASP	O-C-N	5.70	129.94	122.93
1	A	273	GLY	N-CA-C	-5.69	107.25	115.27
1	A	336	ARG	CD-NE-CZ	5.68	132.35	124.40
1	A	306	THR	CB-CA-C	5.67	119.78	110.88
1	A	194	ALA	CA-C-O	5.64	127.13	120.58
1	A	205	ARG	N-CA-CB	5.61	118.56	110.20
1	A	493	SER	CA-C-O	5.60	124.64	118.65
1	A	244	ASN	CA-CB-CG	5.59	118.19	112.60
1	A	262	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	339	ASP	O-C-N	5.59	127.90	122.09
1	A	69	THR	CA-C-O	5.58	125.11	118.69
1	A	13	VAL	N-CA-CB	5.57	118.91	111.90
1	A	209	ASP	O-C-N	5.55	127.79	122.07
1	A	548	ASN	CA-CB-CG	-5.53	107.07	112.60
1	A	20	ASP	O-C-N	5.53	127.98	122.12
1	A	177	THR	CA-C-O	5.52	128.28	121.99
1	A	592	ASN	CA-C-N	5.51	132.06	121.54
1	A	592	ASN	C-N-CA	5.51	132.06	121.54
1	A	396	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	165	ASN	CA-C-O	-5.49	115.22	121.65
1	A	331	ASP	N-CA-CB	5.49	118.05	109.97
1	A	105	ASN	N-CA-C	-5.48	98.65	108.47
1	A	177	THR	CA-C-N	5.48	130.37	121.98
1	A	177	THR	C-N-CA	5.48	130.37	121.98
1	A	280	ARG	N-CA-CB	5.48	117.96	110.01
1	A	22	PHE	CA-C-N	5.48	130.69	122.75
1	A	22	PHE	C-N-CA	5.48	130.69	122.75
1	A	367	ASP	CA-C-O	-5.48	114.89	119.76
1	A	658	SER	N-CA-C	5.47	122.46	110.80
1	A	31	PRO	N-CA-C	-5.47	103.25	111.57
1	A	338	VAL	O-C-N	5.47	127.58	121.94
1	A	105	ASN	CA-C-O	-5.46	115.74	119.29
1	A	14	VAL	CA-C-N	5.45	131.36	123.13
1	A	14	VAL	C-N-CA	5.45	131.36	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	THR	N-CA-C	5.45	117.47	109.24
1	A	152	ARG	CB-CA-C	5.43	118.44	109.70
1	A	133	ALA	CA-C-N	5.42	125.51	119.87
1	A	133	ALA	C-N-CA	5.42	125.51	119.87
1	A	242	ILE	CA-CB-CG2	5.42	119.71	110.50
1	A	371	ARG	NE-CZ-NH1	5.42	126.92	121.50
1	A	607	GLY	N-CA-C	5.41	122.56	115.36
1	A	544	VAL	N-CA-CB	-5.40	102.37	112.36
1	A	633	VAL	N-CA-C	5.40	116.36	108.53
1	A	622	VAL	N-CA-C	5.38	120.54	109.34
1	A	316	GLN	CB-CA-C	5.38	119.44	109.54
1	A	246	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	A	131	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	437	ASN	CA-CB-CG	-5.36	107.24	112.60
1	A	138	SER	O-C-N	5.35	126.09	121.54
1	A	286	ARG	CD-NE-CZ	5.35	131.89	124.40
1	A	669	ASN	OD1-CG-ND2	5.35	127.95	122.60
1	A	261	VAL	CA-C-O	-5.34	114.70	120.36
1	A	402	TYR	N-CA-C	5.34	121.54	114.12
1	A	546	VAL	CB-CA-C	5.34	116.82	110.68
1	A	539	ASN	CA-CB-CG	-5.33	107.27	112.60
1	A	658	SER	O-C-N	5.33	129.68	122.59
1	A	264	ASN	N-CA-CB	5.28	117.98	110.16
1	A	302	MET	N-CA-CB	5.27	117.83	109.82
1	A	203	ILE	O-C-N	5.27	127.07	121.91
1	A	671	THR	O-C-N	5.24	128.81	122.94
1	A	542	ILE	CA-CB-CG2	5.24	119.41	110.50
1	A	543	VAL	CB-CA-C	5.24	118.77	110.81
1	A	29	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	427	LEU	CB-CA-C	5.23	118.27	109.48
1	A	113	ASP	N-CA-C	-5.23	105.48	111.07
1	A	190	LEU	N-CA-C	-5.22	100.58	108.67
1	A	266	HIS	CA-C-N	5.22	127.27	120.28
1	A	266	HIS	C-N-CA	5.22	127.27	120.28
1	A	81	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	200	ASN	O-C-N	5.20	126.48	121.28
1	A	112	SER	O-C-N	5.20	128.08	122.15
1	A	298	GLY	N-CA-C	-5.18	106.49	112.50
1	A	301	GLN	CB-CG-CD	5.17	121.39	112.60
1	A	567	ALA	CA-C-O	-5.17	115.88	121.87
1	A	323	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	36	PHE	CA-C-O	5.13	126.15	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	624	TYR	N-CA-C	-5.13	101.49	109.24
1	A	510	GLN	CB-CG-CD	5.13	121.32	112.60
1	A	411	ASN	CB-CA-C	-5.12	100.16	110.30
1	A	230	MET	CA-C-N	5.12	126.23	119.84
1	A	230	MET	C-N-CA	5.12	126.23	119.84
1	A	411	ASN	OD1-CG-ND2	-5.12	117.48	122.60
1	A	271	GLU	N-CA-C	5.11	120.90	114.31
1	A	441	THR	CA-CB-OG1	-5.10	101.95	109.60
1	A	231	PRO	N-CA-C	5.09	122.96	112.47
1	A	520	THR	CA-C-N	-5.09	114.22	121.50
1	A	520	THR	C-N-CA	-5.09	114.22	121.50
1	A	258	GLU	CA-CB-CG	5.08	124.27	114.10
1	A	657	GLU	CA-C-O	-5.08	116.02	121.56
1	A	20	ASP	CA-C-O	-5.06	115.17	120.63
1	A	417	TYR	CA-C-O	5.06	126.88	121.16
1	A	324	ASP	N-CA-C	5.06	119.45	113.28
1	A	3	ASN	CB-CA-C	5.05	120.17	111.68
1	A	167	ALA	O-C-N	5.04	127.91	122.11
1	A	477	ASP	O-C-N	5.04	129.01	123.16
1	A	549	VAL	CA-C-O	-5.03	116.89	121.72
1	A	352	PRO	N-CA-C	5.03	118.75	110.55
1	A	662	HIS	N-CA-C	-5.01	101.54	109.96

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	5318	0	5029	248	0
2	A	2	0	0	0	0
3	A	231	0	0	14	0
All	All	5551	0	5029	248	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 24.

All (248) 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:592:ASN:HB3	1:A:593:LEU:HD23	1.40	1.03
1:A:137:THR:HG22	1:A:194:ALA:HB3	1.45	0.99
1:A:177:THR:HG22	1:A:188:ARG:HB2	1.44	0.99
1:A:557:THR:HG21	1:A:565:THR:HG23	1.44	0.98
1:A:519:GLY:H	1:A:539:ASN:ND2	1.67	0.93
1:A:519:GLY:N	1:A:539:ASN:HD22	1.66	0.91
1:A:306:THR:CG2	1:A:349:ARG:HH21	1.83	0.91
1:A:306:THR:HG21	1:A:349:ARG:HH21	1.35	0.91
1:A:503:MET:HA	1:A:503:MET:HE2	1.54	0.90
1:A:409:TRP:HB3	1:A:416:VAL:HG13	1.54	0.89
1:A:519:GLY:H	1:A:539:ASN:HD22	0.88	0.88
1:A:258:GLU:HG3	1:A:287:GLN:NE2	1.91	0.86
1:A:618:MET:HE3	1:A:631:ILE:HG22	1.59	0.84
1:A:79:ASN:HD22	1:A:92:SER:HB2	1.44	0.82
1:A:244:ASN:HD22	1:A:509:HIS:HE1	1.27	0.82
1:A:290:ARG:HH11	1:A:291:ASN:HD21	1.28	0.81
1:A:224:MET:HG3	1:A:274:MET:HE2	1.64	0.79
1:A:258:GLU:HG3	1:A:287:GLN:HE21	1.48	0.79
1:A:244:ASN:HD22	1:A:509:HIS:CE1	2.01	0.79
1:A:137:THR:CG2	1:A:194:ALA:HB3	2.13	0.78
1:A:15:TYR:HB3	1:A:71:ILE:HD12	1.66	0.77
1:A:246:ARG:HD3	1:A:246:ARG:C	2.10	0.77
1:A:137:THR:HG23	1:A:138:SER:H	1.50	0.76
1:A:557:THR:CG2	1:A:565:THR:HG23	2.15	0.76
1:A:280:ARG:HD2	3:A:863:HOH:O	1.85	0.75
1:A:583:ARG:HD3	1:A:632:ASP:OD1	1.85	0.75
1:A:239:MET:HE1	1:A:250:THR:HG23	1.69	0.74
1:A:177:THR:HG21	1:A:185:GLY:HA2	1.69	0.74
1:A:64:THR:HG22	1:A:126:ILE:HD11	1.69	0.74
1:A:221:GLY:HA2	1:A:248:VAL:HG13	1.67	0.74
1:A:585:VAL:HB	1:A:675:ILE:HG12	1.69	0.73
1:A:283:GLN:HE21	1:A:283:GLN:HA	1.52	0.73
1:A:419:ARG:HB2	1:A:426:VAL:HG13	1.69	0.73
1:A:185:GLY:O	3:A:912:HOH:O	2.06	0.72
1:A:437:ASN:ND2	1:A:438:TYR:N	2.37	0.72
1:A:385:GLN:HA	1:A:388:GLN:HE21	1.58	0.69
1:A:611:THR:HG21	1:A:654:VAL:HG11	1.74	0.69
1:A:236:LYS:HD2	1:A:504:MET:HE1	1.73	0.69
1:A:510:GLN:HE21	1:A:510:GLN:HA	1.58	0.69
1:A:66:MET:HE2	1:A:387:ILE:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASN:HB2	1:A:414:VAL:H	1.58	0.68
1:A:280:ARG:O	1:A:284:LYS:HB2	1.92	0.68
1:A:340:MET:HE1	1:A:432:ARG:HA	1.75	0.68
1:A:62:TYR:HA	1:A:379:LYS:HE2	1.75	0.68
1:A:649:ASP:CG	1:A:653:ASN:HB2	2.19	0.68
1:A:122:HIS:HE1	1:A:220:ASP:OD2	1.76	0.68
1:A:266:HIS:CE1	1:A:280:ARG:HH21	2.13	0.67
1:A:592:ASN:HB3	1:A:593:LEU:CD2	2.23	0.67
1:A:424:ASP:OD1	1:A:489:SER:HA	1.94	0.67
1:A:239:MET:HE1	1:A:250:THR:CG2	2.25	0.66
1:A:664:TYR:OH	1:A:667:PRO:HD3	1.96	0.66
1:A:177:THR:HG22	1:A:188:ARG:CB	2.25	0.66
1:A:635:VAL:HG22	1:A:636:PRO:HD2	1.76	0.66
1:A:298:GLY:O	1:A:301:GLN:HG2	1.96	0.65
1:A:411:ASN:HB3	1:A:413:ASP:H	1.60	0.65
1:A:137:THR:CG2	1:A:138:SER:H	2.10	0.65
1:A:534:VAL:HB	1:A:544:VAL:HG23	1.79	0.64
1:A:169:MET:HE2	1:A:169:MET:HA	1.80	0.63
1:A:104:PRO:HG3	1:A:111:LEU:HD13	1.80	0.63
1:A:224:MET:HG3	1:A:274:MET:CE	2.28	0.63
1:A:518:PHE:HB2	1:A:539:ASN:HA	1.81	0.63
1:A:227:VAL:HG12	1:A:254:TRP:HB2	1.80	0.62
1:A:416:VAL:HA	1:A:428:VAL:O	1.99	0.62
1:A:522:THR:HA	1:A:537:TRP:CG	2.34	0.62
1:A:557:THR:HG23	1:A:566:SER:O	2.00	0.62
1:A:109:GLY:HA2	3:A:803:HOH:O	1.99	0.62
1:A:649:ASP:HB2	1:A:653:ASN:HB2	1.81	0.62
1:A:35:LEU:HD13	1:A:83:VAL:HG22	1.82	0.61
1:A:79:ASN:ND2	1:A:97:TRP:H	1.98	0.61
1:A:494:THR:HG22	1:A:564:GLN:OE1	2.01	0.61
1:A:290:ARG:NH1	1:A:291:ASN:HD21	1.98	0.61
1:A:227:VAL:HG22	1:A:268:PHE:CZ	2.37	0.60
1:A:557:THR:HG22	1:A:558:VAL:N	2.16	0.60
1:A:503:MET:HA	1:A:503:MET:CE	2.30	0.59
1:A:226:ALA:HB1	1:A:229:HIS:CD2	2.38	0.59
1:A:400:LEU:CD2	1:A:426:VAL:HG11	2.31	0.59
1:A:404:ASP:O	1:A:419:ARG:HD2	2.01	0.59
1:A:79:ASN:HD21	1:A:97:TRP:H	1.49	0.59
1:A:244:ASN:ND2	1:A:509:HIS:HE1	1.98	0.59
1:A:292:ASN:ND2	3:A:729:HOH:O	2.22	0.59
1:A:77:VAL:CG2	1:A:101:PHE:HA	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD23	1:A:320:ILE:HG22	1.84	0.59
1:A:513:ILE:HD12	1:A:542:ILE:CD1	2.33	0.59
1:A:479:GLY:O	1:A:482:GLU:HB2	2.02	0.58
1:A:212:LYS:HE2	1:A:245:TYR:CD1	2.38	0.58
1:A:14:VAL:HG22	1:A:70:ALA:HB3	1.84	0.58
1:A:648:LYS:HA	1:A:653:ASN:O	2.03	0.58
1:A:150:ASN:HB3	1:A:152:ARG:HD3	1.85	0.57
1:A:370:ASN:OD1	1:A:371:ARG:HD2	2.04	0.57
1:A:509:HIS:O	1:A:545:ALA:HA	2.04	0.57
1:A:610:ASP:OD1	1:A:612:SER:HB2	2.04	0.57
1:A:559:GLN:HA	1:A:564:GLN:O	2.04	0.57
1:A:66:MET:HE3	1:A:359:GLU:HG3	1.86	0.57
1:A:552:GLY:HA2	1:A:604:TYR:CE1	2.40	0.57
1:A:17:ILE:HD12	1:A:71:ILE:HG13	1.87	0.56
1:A:226:ALA:HB1	1:A:229:HIS:HD2	1.69	0.56
1:A:177:THR:HB	1:A:184:ASP:OD2	2.06	0.56
1:A:488:TYR:OH	1:A:490:ALA:HB2	2.04	0.56
1:A:557:THR:HG21	1:A:565:THR:CG2	2.26	0.56
1:A:350:GLY:O	1:A:394:ARG:NH2	2.39	0.56
1:A:77:VAL:HG21	1:A:101:PHE:HA	1.87	0.56
1:A:302:MET:O	1:A:306:THR:HB	2.07	0.55
1:A:637:GLU:HB2	1:A:668:THR:HA	1.89	0.55
1:A:44:ARG:HD2	1:A:88:SER:CB	2.37	0.55
1:A:389:LYS:HE3	1:A:459:LEU:HD22	1.89	0.55
1:A:553:LYS:HE2	1:A:573:GLU:HB2	1.87	0.55
1:A:620:ASN:HD22	1:A:620:ASN:C	2.15	0.54
1:A:178:THR:HG22	1:A:180:SER:OG	2.07	0.54
1:A:51:TRP:CZ3	1:A:114:PHE:HB2	2.42	0.54
1:A:306:THR:HG21	1:A:349:ARG:NH2	2.13	0.54
1:A:649:ASP:CB	1:A:653:ASN:HB2	2.37	0.54
1:A:410:ILE:HA	1:A:414:VAL:O	2.08	0.54
1:A:204:ASP:OD1	1:A:208:LYS:NZ	2.36	0.54
1:A:254:TRP:CE2	1:A:265:ASN:HB2	2.43	0.54
1:A:19:VAL:HG23	1:A:74:SER:OG	2.07	0.53
1:A:94:HIS:ND1	1:A:96:TYR:HB2	2.23	0.53
1:A:664:TYR:HB2	1:A:674:ILE:HD13	1.88	0.53
1:A:75:GLN:HA	1:A:131:ASP:O	2.08	0.53
1:A:416:VAL:HB	1:A:429:ALA:HA	1.90	0.53
1:A:138:SER:HB2	1:A:139:PRO:CD	2.38	0.53
1:A:615:ILE:HD12	1:A:615:ILE:N	2.24	0.53
1:A:411:ASN:CB	1:A:414:VAL:H	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:TRP:CG	1:A:415:TYR:HB2	2.45	0.52
1:A:542:ILE:C	1:A:542:ILE:HD13	2.35	0.52
1:A:9:PHE:CE2	1:A:129:ILE:HD11	2.45	0.52
1:A:22:PHE:HB3	3:A:700:HOH:O	2.10	0.52
1:A:138:SER:HB2	1:A:139:PRO:HD2	1.91	0.52
1:A:592:ASN:HB2	1:A:595:GLN:OE1	2.10	0.51
1:A:615:ILE:HG22	1:A:631:ILE:HD13	1.90	0.51
1:A:639:LYS:NZ	3:A:831:HOH:O	2.43	0.51
1:A:1:ALA:HB2	1:A:123:ALA:O	2.11	0.51
1:A:55:ILE:HG13	1:A:117:LEU:HD12	1.93	0.51
1:A:558:VAL:O	1:A:565:THR:HA	2.11	0.51
1:A:16:GLN:HG3	1:A:72:TRP:CD2	2.45	0.51
1:A:648:LYS:HG3	1:A:654:VAL:HG22	1.91	0.51
1:A:641:ILE:HG12	1:A:664:TYR:O	2.11	0.51
1:A:300:ASN:HD21	1:A:407:GLN:HB2	1.76	0.50
1:A:306:THR:HG23	1:A:349:ARG:HH21	1.73	0.50
1:A:21:ARG:C	1:A:373:MET:HE3	2.37	0.50
1:A:593:LEU:CG	1:A:594:GLY:H	2.24	0.50
1:A:496:ILE:HG22	3:A:706:HOH:O	2.10	0.50
1:A:1:ALA:HB1	3:A:834:HOH:O	2.12	0.50
1:A:326:ASP:HB3	1:A:365:ASN:ND2	2.26	0.50
1:A:497:ILE:HD11	1:A:558:VAL:HG23	1.94	0.50
1:A:84:MET:HG2	1:A:85:ASN:H	1.77	0.49
1:A:397:ASN:ND2	1:A:487:ALA:HB1	2.26	0.49
1:A:227:VAL:CG1	1:A:254:TRP:HB2	2.42	0.49
1:A:18:VAL:HG13	1:A:356:TYR:CE1	2.47	0.49
1:A:137:THR:HG21	1:A:151:GLY:O	2.13	0.49
1:A:299:PHE:O	1:A:303:ILE:HG12	2.12	0.49
1:A:248:VAL:HG12	1:A:250:THR:HG22	1.95	0.49
1:A:122:HIS:HD2	3:A:766:HOH:O	1.95	0.49
1:A:258:GLU:CG	1:A:287:GLN:HE21	2.20	0.49
1:A:455:GLN:N	1:A:485:VAL:O	2.33	0.48
1:A:6:LYS:HG2	1:A:220:ASP:HA	1.96	0.48
1:A:23:VAL:O	1:A:49:GLY:HA2	2.13	0.48
1:A:283:GLN:HE21	1:A:283:GLN:CA	2.25	0.48
1:A:5:ASN:ND2	1:A:8:ASN:HB3	2.29	0.48
1:A:585:VAL:CB	1:A:675:ILE:HG12	2.40	0.48
1:A:57:LYS:HE2	1:A:377:PHE:CD1	2.48	0.47
1:A:486:TRP:HA	3:A:865:HOH:O	2.14	0.47
1:A:287:GLN:O	1:A:292:ASN:N	2.48	0.47
1:A:454:ASP:OD1	1:A:456:LEU:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:HG3	1:A:368:PRO:HG3	1.97	0.47
1:A:84:MET:HE2	1:A:147:TYR:OH	2.15	0.47
1:A:642:GLU:HA	1:A:662:HIS:O	2.14	0.47
1:A:438:TYR:O	1:A:477:ASP:HA	2.14	0.47
1:A:513:ILE:HD12	1:A:542:ILE:HD12	1.96	0.47
1:A:137:THR:HG23	1:A:138:SER:N	2.24	0.47
1:A:553:LYS:CD	1:A:573:GLU:HB2	2.45	0.46
1:A:606:LEU:HD11	1:A:633:VAL:HG11	1.97	0.46
1:A:66:MET:CE	1:A:387:ILE:HD13	2.45	0.46
1:A:522:THR:HA	1:A:537:TRP:CD1	2.51	0.46
1:A:223:ARG:C	1:A:223:ARG:HD2	2.40	0.46
1:A:615:ILE:HG21	1:A:633:VAL:HG22	1.97	0.46
1:A:374:MET:HG2	1:A:377:PHE:CZ	2.51	0.45
1:A:400:LEU:HD21	1:A:426:VAL:HG11	1.97	0.45
1:A:12:ASP:OD2	1:A:69:THR:HG22	2.15	0.45
1:A:522:THR:HA	1:A:537:TRP:CD2	2.51	0.45
1:A:375:SER:OG	1:A:376:SER:N	2.50	0.45
1:A:69:THR:O	1:A:126:ILE:HA	2.17	0.45
1:A:389:LYS:HE3	1:A:456:LEU:O	2.17	0.45
1:A:530:THR:HA	3:A:828:HOH:O	2.17	0.45
1:A:69:THR:HG23	3:A:688:HOH:O	2.16	0.45
1:A:294:ASP:OD1	1:A:295:ASN:N	2.46	0.45
1:A:326:ASP:HB3	1:A:365:ASN:HD22	1.81	0.45
1:A:20:ASP:CG	1:A:47:CYS:H	2.22	0.45
1:A:184:ASP:O	1:A:188:ARG:HB2	2.17	0.44
1:A:223:ARG:HA	1:A:251:PHE:O	2.18	0.44
1:A:534:VAL:HA	1:A:544:VAL:HG23	1.98	0.44
1:A:17:ILE:HD11	1:A:71:ILE:HD11	1.99	0.44
1:A:425:VAL:O	1:A:488:TYR:N	2.45	0.44
1:A:488:TYR:CZ	1:A:490:ALA:HB2	2.52	0.44
1:A:242:ILE:HD13	1:A:250:THR:HG21	1.98	0.44
1:A:437:ASN:ND2	1:A:437:ASN:C	2.75	0.44
1:A:441:THR:HG22	1:A:475:ALA:HB2	1.99	0.44
1:A:262:ASP:OD1	1:A:264:ASN:N	2.48	0.44
1:A:657:GLU:OE2	1:A:662:HIS:NE2	2.34	0.44
1:A:270:ASN:HD21	1:A:310:TYR:HA	1.83	0.44
1:A:419:ARG:O	1:A:425:VAL:HA	2.18	0.44
1:A:526:LYS:O	1:A:556:ILE:HA	2.18	0.44
1:A:72:TRP:CD1	1:A:72:TRP:C	2.95	0.44
1:A:43:LEU:HD11	1:A:372:LYS:HA	1.99	0.43
1:A:44:ARG:HD2	1:A:88:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASN:HD22	1:A:105:ASN:C	2.26	0.43
1:A:420:GLN:HA	1:A:424:ASP:O	2.18	0.43
1:A:620:ASN:O	1:A:625:SER:HA	2.17	0.43
1:A:160:LEU:O	1:A:170:TYR:HE2	2.00	0.43
1:A:227:VAL:HG21	1:A:252:GLY:HA3	2.00	0.43
1:A:138:SER:CB	1:A:139:PRO:CD	2.96	0.43
1:A:59:ASN:N	1:A:59:ASN:HD22	2.15	0.43
1:A:500:VAL:HB	1:A:503:MET:HE3	2.01	0.43
1:A:66:MET:HE2	1:A:387:ILE:CD1	2.45	0.43
1:A:514:ASP:OD1	1:A:541:GLN:HG3	2.19	0.43
1:A:20:ASP:OD2	1:A:47:CYS:N	2.46	0.42
1:A:533:ASN:O	1:A:544:VAL:HG22	2.19	0.42
1:A:142:GLU:OE1	1:A:173:HIS:HD2	2.02	0.42
1:A:266:HIS:CE1	1:A:280:ARG:NH2	2.85	0.42
1:A:649:ASP:OD1	1:A:653:ASN:HB2	2.19	0.42
1:A:447:LEU:HA	1:A:448:PRO:HD3	1.89	0.42
1:A:513:ILE:O	1:A:541:GLN:HA	2.20	0.42
1:A:244:ASN:ND2	1:A:509:HIS:CE1	2.76	0.42
1:A:284:LYS:HE3	1:A:294:ASP:OD2	2.20	0.42
1:A:536:SER:O	1:A:542:ILE:HA	2.20	0.42
1:A:559:GLN:HB2	1:A:565:THR:OG1	2.20	0.42
1:A:518:PHE:HB2	1:A:539:ASN:CA	2.48	0.42
1:A:642:GLU:HG2	1:A:663:VAL:HG22	2.01	0.42
1:A:527:PHE:CZ	1:A:546:VAL:HG22	2.55	0.41
1:A:50:ASP:HB2	3:A:908:HOH:O	2.21	0.41
1:A:166:ASP:O	1:A:167:ALA:C	2.63	0.41
1:A:664:TYR:CD1	1:A:674:ILE:HD12	2.55	0.41
1:A:33:GLY:C	1:A:35:LEU:H	2.29	0.41
1:A:217:MET:HE3	1:A:217:MET:HB3	2.01	0.41
1:A:302:MET:HE3	1:A:302:MET:HB3	1.91	0.41
1:A:421:PHE:CE1	1:A:498:GLY:HA2	2.56	0.41
1:A:478:LEU:HD12	1:A:478:LEU:HA	1.80	0.41
1:A:542:ILE:HD11	1:A:544:VAL:HB	2.02	0.41
1:A:664:TYR:CE2	1:A:666:THR:HA	2.56	0.41
1:A:111:LEU:O	1:A:114:PHE:HB3	2.21	0.41
1:A:200:ASN:HD22	1:A:200:ASN:C	2.29	0.40
1:A:62:TYR:HD1	1:A:379:LYS:HE3	1.85	0.40
1:A:258:GLU:HA	1:A:283:GLN:HB3	2.03	0.40
1:A:593:LEU:HA	3:A:886:HOH:O	2.20	0.40
1:A:116:ARG:HH11	1:A:116:ARG:HD2	1.62	0.40
1:A:67:GLY:HA3	1:A:391:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TRP:NE1	1:A:265:ASN:HB2	2.36	0.40
1:A:619:PHE:O	1:A:629:TRP:HA	2.21	0.40
1:A:620:ASN:HB2	1:A:626:TYR:HB2	2.03	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	678/680 (100%)	633 (93%)	41 (6%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	PHE
1	A	593	LEU
1	A	19	VAL
1	A	622	VAL

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	578/578 (100%)	471 (82%)	107 (18%)	1	3

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	4	LEU
1	A	6	LYS
1	A	7	VAL
1	A	11	SER
1	A	18	VAL
1	A	27	THR
1	A	35	LEU
1	A	38	SER
1	A	42	ASN
1	A	43	LEU
1	A	63	LEU
1	A	71	ILE
1	A	77	VAL
1	A	83	VAL
1	A	103	LYS
1	A	105	ASN
1	A	111	LEU
1	A	116	ARG
1	A	137	THR
1	A	138	SER
1	A	143	THR
1	A	146	SER
1	A	156	ASN
1	A	159	LEU
1	A	169	MET
1	A	177	THR
1	A	178	THR
1	A	180	SER
1	A	193	LEU
1	A	199	GLN
1	A	200	ASN
1	A	207	LEU
1	A	208	LYS
1	A	212	LYS
1	A	227	VAL
1	A	242	ILE
1	A	246	ARG
1	A	248	VAL
1	A	250	THR
1	A	256	LEU
1	A	257	SER

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Mol	Chain	Res	Type
1	A	265	ASN
1	A	274	MET
1	A	280	ARG
1	A	283	GLN
1	A	284	LYS
1	A	290	ARG
1	A	292	ASN
1	A	293	SER
1	A	306	THR
1	A	314	LEU
1	A	330	ILE
1	A	342	LEU
1	A	345	LEU
1	A	346	LEU
1	A	368	PRO
1	A	371	ARG
1	A	381	THR
1	A	386	VAL
1	A	393	LEU
1	A	395	ARG
1	A	405	THR
1	A	406	GLU
1	A	407	GLN
1	A	411	ASN
1	A	416	VAL
1	A	425	VAL
1	A	426	VAL
1	A	428	VAL
1	A	430	VAL
1	A	459	LEU
1	A	477	ASP
1	A	482	GLU
1	A	493	SER
1	A	507	VAL
1	A	510	GLN
1	A	520	THR
1	A	522	THR
1	A	524	THR
1	A	529	THR
1	A	534	VAL
1	A	542	ILE
1	A	543	VAL

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Mol	Chain	Res	Type
1	A	544	VAL
1	A	550	SER
1	A	561	SER
1	A	562	SER
1	A	580	VAL
1	A	583	ARG
1	A	592	ASN
1	A	593	LEU
1	A	599	ILE
1	A	600	VAL
1	A	602	ASN
1	A	603	VAL
1	A	606	LEU
1	A	620	ASN
1	A	635	VAL
1	A	639	LYS
1	A	649	ASP
1	A	655	THR
1	A	658	SER
1	A	660	SER
1	A	668	THR
1	A	669	ASN
1	A	673	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	42	ASN
1	A	56	ASN
1	A	59	ASN
1	A	79	ASN
1	A	105	ASN
1	A	122	HIS
1	A	156	ASN
1	A	165	ASN
1	A	173	HIS
1	A	200	ASN
1	A	235	GLN
1	A	270	ASN
1	A	283	GLN
1	A	291	ASN

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Mol	Chain	Res	Type
1	A	300	ASN
1	A	304	GLN
1	A	365	ASN
1	A	388	GLN
1	A	396	ASN
1	A	397	ASN
1	A	420	GLN
1	A	466	GLN
1	A	474	ASN
1	A	509	HIS
1	A	510	GLN
1	A	521	ASN
1	A	533	ASN
1	A	539	ASN
1	A	540	ASN
1	A	559	GLN
1	A	577	ASN
1	A	579	GLN
1	A	592	ASN
1	A	602	ASN
1	A	608	ASN
1	A	620	ASN
1	A	651	GLN
1	A	653	ASN
1	A	669	ASN
1	A	679	GLN
1	A	680	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	680/680 (100%)	-0.49	1 (0%) 92 90	6, 12, 21, 34	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	594	GLY	3.6

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	CA	A	681	1/1	0.63	0.14	9,9,9,9	0
2	CA	A	682	1/1	0.95	0.02	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.