



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:24 PM UTC

PDB ID : 1GUP / pdb_00001gup
Title : STRUCTURE OF NUCLEOTIDYLTRANSFERASE COMPLEXED WITH
UDP-GALACTOSE
Authors : Thoden, J.B.; Rayment, I.; Holden, H.
Deposited on : 1996-10-23
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

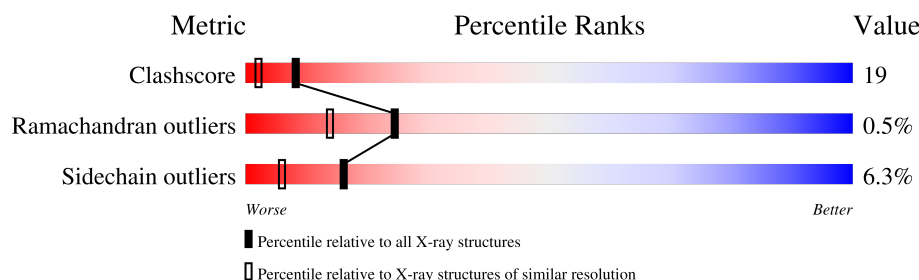
1 Overall quality at a glance

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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	 64% 29% 6%
1	B	348	 59% 34% 6% .
1	C	348	 57% 34% 7% ..
1	D	348	 51% 41% 7% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12487 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.

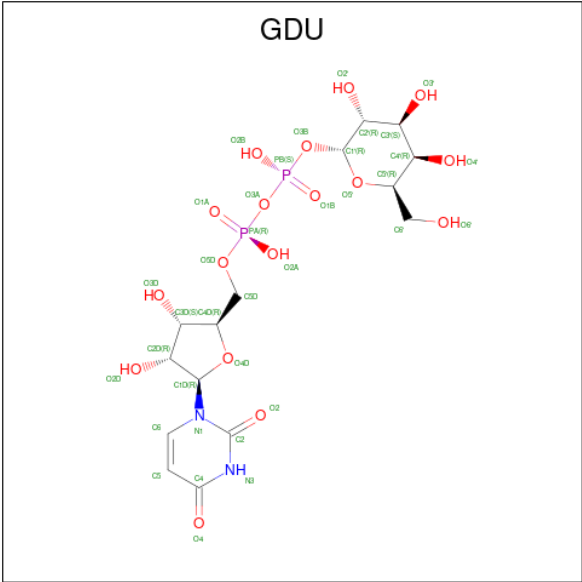
- Molecule 1 is a protein called GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2784	1763	492	516	13			
1	B	344	Total	C	N	O	S	0	0	0
			2766	1753	489	511	13			
1	C	344	Total	C	N	O	S	0	0	0
			2766	1753	489	511	13			
1	D	344	Total	C	N	O	S	0	0	0
			2766	1753	489	511	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	GLY	HIS	engineered mutation	UNP P09148
B	166	GLY	HIS	engineered mutation	UNP P09148
C	166	GLY	HIS	engineered mutation	UNP P09148
D	166	GLY	HIS	engineered mutation	UNP P09148

- Molecule 2 is GALACTOSE-URIDINE-5'-DIPHOSPHATE (CCD ID: GDU) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
2	D	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Fe 1	0	0
4	C	1	Total 1	Fe 1	0	0
4	D	1	Total 1	Fe 1	0	0

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	K 1	0	0
5	B	1	Total 1	K 1	0	0
5	C	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0

- Molecule 6 is water.

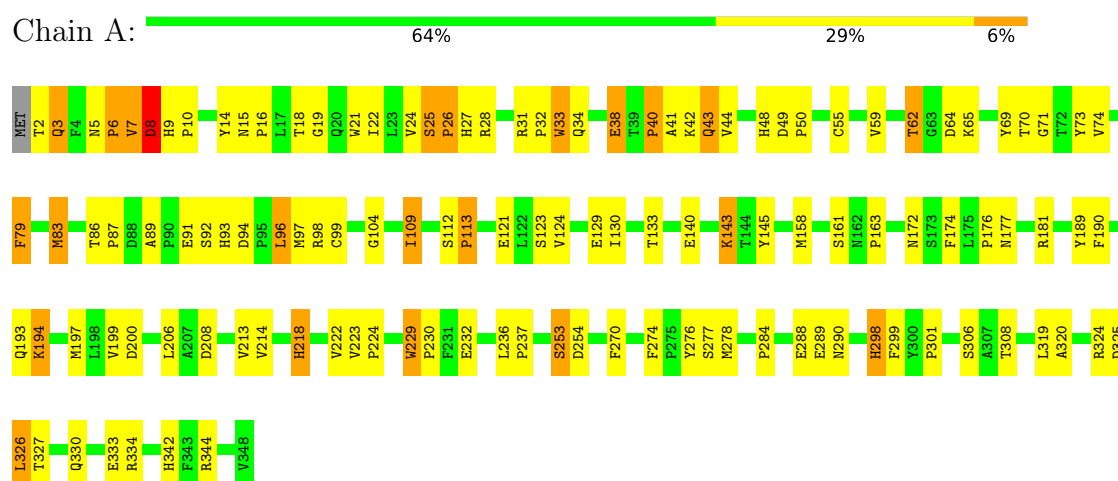
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	371	Total 371	O 371	0	0
6	B	330	Total 330	O 330	0	0
6	C	291	Total 291	O 291	0	0
6	D	257	Total 257	O 257	0	0

3 Residue-property plots [i](#)

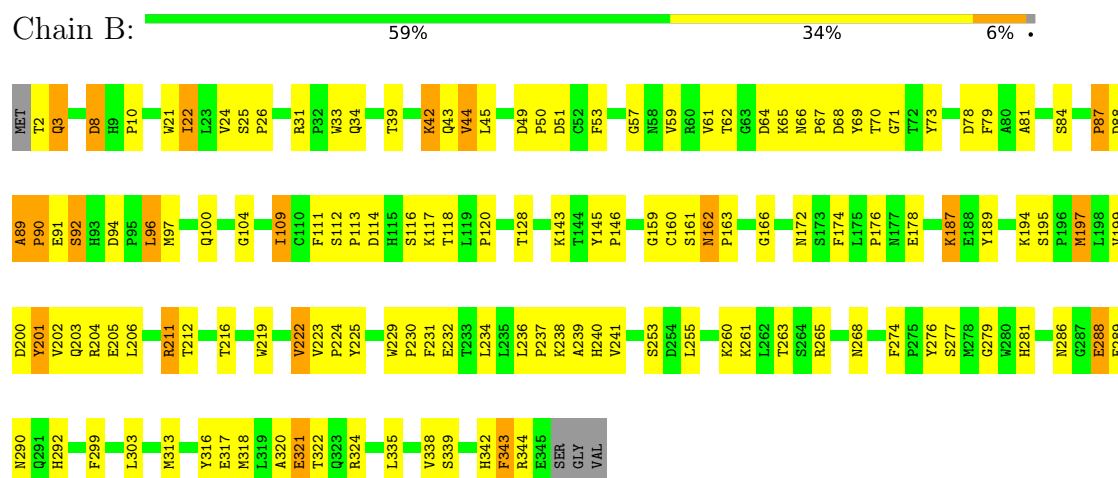
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE

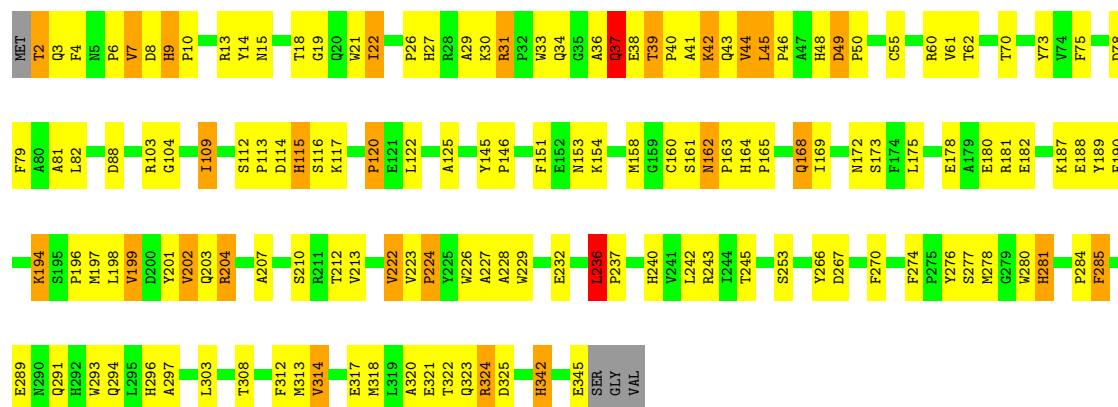


• Molecule 1: GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE



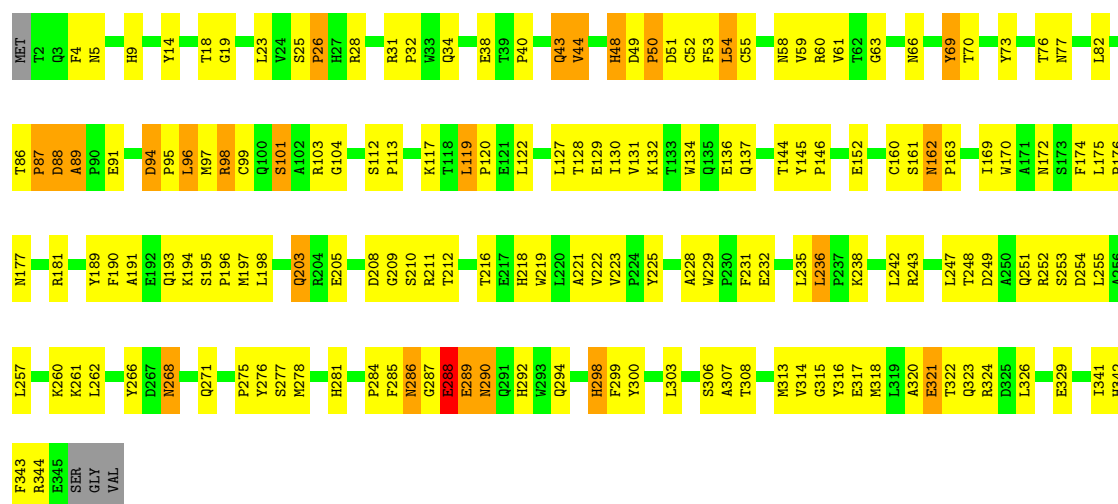
• Molecule 1: GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE





• Molecule 1: GALACTOSE-1-PHOSPHATE URIDYLTRANSFERASE

Chain D: 51% 41% 7% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.70Å 57.70Å 188.70Å 90.00° 100.08° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (30.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.191 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12487	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, K, GDU, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.18	3/2869 (0.1%)	1.67	35/3912 (0.9%)
1	B	1.12	1/2851 (0.0%)	1.67	46/3889 (1.2%)
1	C	1.09	4/2851 (0.1%)	1.69	52/3889 (1.3%)
1	D	1.06	1/2851 (0.0%)	1.64	40/3889 (1.0%)
All	All	1.12	9/11422 (0.1%)	1.67	173/15579 (1.1%)

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	C	1	0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180	GLU	CD-OE1	6.26	1.37	1.25
1	A	130	ILE	CA-CB	-6.06	1.47	1.54
1	C	60	ARG	NE-CZ	5.41	1.39	1.33
1	D	28	ARG	CZ-NH1	5.30	1.40	1.32
1	B	78	ASP	CG-OD2	5.27	1.35	1.25
1	A	129	GLU	CD-OE1	5.21	1.35	1.25
1	C	175	LEU	CA-CB	5.13	1.60	1.53
1	A	333	GLU	CD-OE2	5.09	1.35	1.25
1	C	182	GLU	CD-OE2	5.02	1.34	1.25

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	ILE	CB-CA-C	-11.45	93.61	110.33
1	C	88	ASP	CA-CB-CG	10.98	123.58	112.60
1	C	213	VAL	CB-CA-C	9.52	120.44	111.30
1	B	51	ASP	CA-CB-CG	-9.47	103.13	112.60
1	D	175	LEU	CB-CA-C	-9.29	100.97	110.17
1	B	89	ALA	N-CA-CB	9.20	119.88	109.49
1	C	224	PRO	N-CA-CB	8.94	112.64	103.25
1	A	96	LEU	N-CA-CB	8.64	125.48	110.44
1	A	59	VAL	N-CA-CB	8.39	122.13	110.56
1	D	321	GLU	N-CA-CB	-8.28	98.72	111.56
1	D	254	ASP	CA-CB-CG	-8.03	104.57	112.60
1	C	37	GLN	N-CA-CB	8.03	123.62	110.37
1	C	103	ARG	N-CA-CB	7.98	123.02	111.05
1	C	281	HIS	CA-CB-CG	-7.97	105.83	113.80
1	B	87	PRO	N-CA-CB	7.75	110.21	103.31
1	D	342	HIS	CA-CB-CG	-7.67	106.13	113.80
1	C	289	GLU	N-CA-CB	7.49	121.56	109.95
1	D	89	ALA	N-CA-C	-7.48	100.66	110.39
1	C	175	LEU	CB-CA-C	-7.47	102.77	110.17
1	D	285	PHE	N-CA-CB	7.42	118.66	110.35
1	B	224	PRO	N-CA-CB	7.29	109.45	103.32
1	D	87	PRO	CB-CA-C	-7.24	101.47	110.95
1	B	94	ASP	CA-CB-CG	-7.18	105.42	112.60
1	C	42	LYS	N-CA-C	7.12	120.03	110.35
1	A	223	VAL	N-CA-CB	7.00	121.02	111.21
1	D	196	PRO	N-CA-CB	6.99	109.51	103.36
1	D	40	PRO	N-CA-CB	6.97	109.94	103.39
1	A	284	PRO	CB-CA-C	-6.93	101.90	110.98
1	C	62	THR	CB-CA-C	-6.91	98.88	110.56
1	A	181	ARG	CD-NE-CZ	-6.86	114.80	124.40
1	B	8	ASP	CA-CB-CG	6.86	119.45	112.60
1	A	224	PRO	N-CA-CB	6.84	109.06	103.32
1	D	289	GLU	N-CA-CB	6.80	121.60	110.17
1	A	290	ASN	CA-CB-CG	-6.79	105.81	112.60
1	B	160	CYS	N-CA-C	-6.77	100.46	110.48
1	A	277	SER	N-CA-CB	6.75	122.02	110.68
1	B	62	THR	N-CA-CB	-6.72	100.75	110.56
1	B	231	PHE	CA-CB-CG	-6.60	107.20	113.80
1	C	196	PRO	N-CA-CB	6.58	109.16	103.36
1	C	9	HIS	N-CA-C	6.58	117.94	109.65
1	D	162	ASN	CA-C-N	6.55	126.25	119.64
1	D	162	ASN	C-N-CA	6.55	126.25	119.64
1	D	96	LEU	N-CA-CB	6.51	120.38	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	94	ASP	CA-CB-CG	-6.50	106.10	112.60
1	C	199	VAL	N-CA-C	-6.49	104.43	110.53
1	B	162	ASN	CA-CB-CG	6.46	119.06	112.60
1	D	277	SER	N-CA-CB	6.46	121.98	110.80
1	D	44	VAL	N-CA-C	6.46	116.69	106.88
1	B	25	SER	CA-C-N	6.40	127.84	119.84
1	B	25	SER	C-N-CA	6.40	127.84	119.84
1	C	115	HIS	N-CA-CB	-6.36	100.09	110.14
1	B	324	ARG	N-CA-CB	6.27	120.38	110.23
1	D	25	SER	CA-C-N	6.26	127.67	119.84
1	D	25	SER	C-N-CA	6.26	127.67	119.84
1	D	290	ASN	CA-CB-CG	-6.26	106.34	112.60
1	B	222	VAL	CB-CA-C	-6.24	101.58	110.82
1	A	298	HIS	CA-CB-CG	6.24	120.04	113.80
1	A	190	PHE	CA-CB-CG	-6.21	107.59	113.80
1	B	44	VAL	N-CA-C	6.17	116.75	107.80
1	D	69	TYR	N-CA-C	6.16	118.67	110.53
1	B	299	PHE	N-CA-CB	6.15	120.42	110.77
1	B	117	LYS	N-CA-C	6.13	118.28	108.41
1	D	223	VAL	N-CA-C	-6.13	95.64	108.88
1	D	288	GLU	N-CA-C	6.10	118.58	110.53
1	B	199	VAL	N-CA-C	-6.08	104.92	110.82
1	C	314	VAL	N-CA-CB	-6.07	105.33	112.32
1	B	39	THR	CB-CA-C	6.06	118.62	110.13
1	C	236	LEU	O-C-N	6.03	126.16	121.88
1	C	44	VAL	CB-CA-C	6.00	121.13	111.29
1	C	10	PRO	N-CA-CB	5.99	108.89	103.19
1	C	303	LEU	N-CA-CB	5.97	118.84	109.83
1	D	286	ASN	CB-CA-C	5.96	120.76	109.37
1	A	208	ASP	CA-CB-CG	5.95	118.55	112.60
1	D	281	HIS	CA-CB-CG	-5.94	107.86	113.80
1	C	78	ASP	CA-CB-CG	-5.93	106.67	112.60
1	B	68	ASP	CA-CB-CG	5.93	118.53	112.60
1	C	236	LEU	CB-CA-C	5.92	118.69	108.91
1	C	42	LYS	N-CA-CB	5.89	118.70	110.04
1	C	9	HIS	CA-CB-CG	-5.88	107.92	113.80
1	D	231	PHE	CA-CB-CG	-5.88	107.92	113.80
1	D	44	VAL	N-CA-CB	-5.88	104.55	111.60
1	A	18	THR	N-CA-CB	-5.87	103.09	110.90
1	A	223	VAL	N-CA-C	-5.87	96.20	108.88
1	C	202	VAL	CB-CA-C	-5.82	104.52	111.97
1	C	285	PHE	N-CA-CB	5.81	117.03	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	VAL	CB-CA-C	5.81	119.63	112.02
1	B	277	SER	N-CA-CB	5.81	120.44	110.68
1	C	49	ASP	CB-CA-C	5.79	118.24	110.13
1	A	222	VAL	CB-CA-C	-5.79	102.25	110.82
1	D	73	TYR	N-CA-CB	5.79	120.20	110.77
1	B	84	SER	CB-CA-C	-5.77	99.60	110.67
1	B	59	VAL	N-CA-CB	-5.71	104.49	111.00
1	D	160	CYS	N-CA-C	-5.70	100.70	109.76
1	D	170	TRP	CB-CA-C	-5.70	101.57	110.74
1	A	218	HIS	N-CA-CB	-5.65	102.08	110.61
1	C	222	VAL	N-CA-CB	-5.63	105.84	112.32
1	A	79	PHE	CA-CB-CG	-5.62	108.18	113.80
1	C	270	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	62	THR	CB-CA-C	-5.59	100.41	110.37
1	D	298	HIS	CB-CA-C	-5.59	98.70	109.37
1	A	199	VAL	N-CA-C	-5.58	105.09	110.72
1	D	63	GLY	N-CA-C	-5.58	107.67	114.92
1	D	275	PRO	N-CA-CB	5.57	109.22	103.38
1	B	64	ASP	CA-CB-CG	5.55	118.16	112.60
1	B	276	TYR	CB-CA-C	-5.55	100.12	110.56
1	A	158	MET	N-CA-CB	5.55	119.79	110.92
1	A	93	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	237	PRO	N-CA-CB	5.54	108.52	103.15
1	A	230	PRO	N-CA-CB	5.54	109.06	103.25
1	B	178	GLU	N-CA-CB	5.52	118.34	110.06
1	C	44	VAL	N-CA-CB	5.51	120.32	111.23
1	C	178	GLU	N-CA-CB	5.50	118.80	110.28
1	B	53	PHE	N-CA-CB	5.50	118.68	110.22
1	C	196	PRO	CA-N-CD	-5.48	104.32	112.00
1	C	222	VAL	CB-CA-C	-5.48	102.91	110.91
1	B	90	PRO	N-CA-CB	5.46	106.89	103.23
1	D	268	ASN	CA-CB-CG	-5.46	107.14	112.60
1	B	201	TYR	CB-CA-C	-5.45	102.08	110.81
1	C	342	HIS	CA-CB-CG	-5.45	108.35	113.80
1	C	39	THR	CB-CA-C	5.44	119.57	110.97
1	D	25	SER	O-C-N	5.43	125.78	121.17
1	A	274	PHE	CA-CB-CG	5.42	119.22	113.80
1	A	86	THR	CA-CB-OG1	-5.42	101.47	109.60
1	A	113	PRO	N-CA-CB	5.41	108.50	103.41
1	A	33	TRP	N-CA-CB	5.41	119.61	110.46
1	C	160	CYS	N-CA-CB	5.41	117.96	110.17
1	C	277	SER	N-CA-CB	5.37	120.18	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	277	SER	N-CA-C	-5.36	100.66	109.40
1	A	334	ARG	N-CA-CB	5.33	118.43	110.22
1	C	62	THR	CA-C-N	-5.32	114.96	123.31
1	C	62	THR	C-N-CA	-5.32	114.96	123.31
1	A	181	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	C	158	MET	N-CA-CB	5.31	117.89	110.56
1	C	317	GLU	CA-CB-CG	-5.31	103.49	114.10
1	C	151	PHE	N-CA-C	5.31	116.06	108.74
1	C	229	TRP	CA-CB-CG	-5.30	103.53	113.60
1	B	237	PRO	N-CA-CB	5.30	108.26	103.33
1	B	274	PHE	N-CA-CB	-5.30	102.48	110.32
1	A	25	SER	CA-C-N	5.29	126.46	119.84
1	A	25	SER	C-N-CA	5.29	126.46	119.84
1	B	318	MET	CG-SD-CE	-5.29	89.27	100.90
1	D	54	LEU	CA-C-O	5.29	125.17	119.15
1	B	8	ASP	N-CA-CB	-5.28	103.00	110.81
1	C	13	ARG	N-CA-CB	5.27	119.17	110.69
1	B	281	HIS	CA-CB-CG	-5.27	108.53	113.80
1	B	240	HIS	CB-CA-C	-5.25	102.38	110.26
1	D	306	SER	N-CA-CB	-5.25	103.32	111.35
1	A	334	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	B	223	VAL	N-CA-C	-5.24	97.55	108.88
1	B	109	ILE	N-CA-CB	5.24	118.45	111.64
1	C	162	ASN	CA-CB-CG	5.22	117.82	112.60
1	D	341	ILE	N-CA-CB	5.21	117.24	110.99
1	C	109	ILE	CA-CB-CG2	5.20	119.34	110.50
1	B	26	PRO	N-CA-C	5.20	123.18	112.47
1	A	8	ASP	N-CA-CB	5.20	117.81	110.90
1	A	40	PRO	N-CA-CB	5.20	108.16	103.33
1	D	26	PRO	CA-N-CD	-5.17	104.76	112.00
1	B	84	SER	N-CA-C	5.16	117.80	111.82
1	B	118	THR	N-CA-CB	5.16	117.27	110.25
1	A	87	PRO	CB-CA-C	-5.15	104.23	110.98
1	D	117	LYS	N-CA-C	5.15	117.12	108.73
1	C	120	PRO	N-CA-CB	5.13	108.63	103.25
1	B	96	LEU	N-CA-CB	5.12	119.35	110.44
1	C	210	SER	N-CA-C	5.11	117.75	111.82
1	B	339	SER	N-CA-CB	-5.10	103.07	110.36
1	D	48	HIS	N-CA-CB	5.10	120.22	111.00
1	C	324	ARG	N-CA-CB	5.09	118.92	110.63
1	C	168	GLN	N-CA-CB	-5.08	103.39	111.62
1	A	229	TRP	CA-CB-CG	-5.05	104.00	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	HIS	N-CA-CB	5.04	118.52	110.65
1	B	88	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	44	VAL	CB-CA-C	5.01	118.28	110.96
1	B	230	PRO	N-CA-CB	5.00	108.50	103.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	44	VAL	CA

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	2784	0	2661	104	0
1	B	2766	0	2644	104	0
1	C	2766	0	2644	120	0
1	D	2766	0	2644	144	0
2	A	36	0	22	0	0
2	B	36	0	22	1	0
2	C	36	0	22	0	0
2	D	36	0	22	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	371	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	330	0	0	15	0
6	C	291	0	0	12	1
6	D	257	0	0	8	0
All	All	12487	0	10681	422	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (422) 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:D:61:VAL:HG12	2:D:352:GDU:O4	1.62	1.00
1:D:98:ARG:HG2	1:D:98:ARG:HH11	1.33	0.91
1:C:9:HIS:HD2	1:D:87:PRO:HD2	1.41	0.86
1:B:42:LYS:H	1:B:42:LYS:HD2	1.40	0.85
1:C:33:TRP:CZ3	1:D:161:SER:HB3	2.11	0.85
1:C:154:LYS:HE2	1:C:274:PHE:O	1.79	0.83
1:C:7:VAL:HG13	6:C:797:HOH:O	1.80	0.81
1:A:43:GLN:HG3	1:A:43:GLN:O	1.79	0.81
1:A:253:SER:HB3	6:A:637:HOH:O	1.80	0.81
1:C:33:TRP:CE3	1:D:161:SER:HB3	2.17	0.79
1:D:52:CYS:HB3	1:D:55:CYS:HB2	1.66	0.78
1:D:43:GLN:HB3	1:D:344:ARG:HH12	1.49	0.78
1:B:203:GLN:HB2	6:B:644:HOH:O	1.85	0.77
1:D:236:LEU:HD12	1:D:236:LEU:N	1.98	0.76
1:A:3:GLN:HA	1:A:3:GLN:HE21	1.49	0.76
1:A:9:HIS:CE1	1:B:87:PRO:HG2	2.21	0.76
1:C:145:TYR:HB3	1:C:172:ASN:O	1.84	0.76
1:B:216:THR:O	1:B:238:LYS:NZ	2.19	0.76
1:A:5:ASN:OD1	1:A:7:VAL:HG23	1.84	0.76
1:B:187:LYS:NZ	1:B:187:LYS:HB3	2.01	0.75
1:B:92:SER:HB2	6:B:638:HOH:O	1.86	0.75
1:D:14:TYR:CZ	1:D:19:GLY:HA2	2.22	0.74
1:A:5:ASN:ND2	1:A:8:ASP:OD2	2.19	0.74
1:B:89:ALA:HB1	1:B:90:PRO:HD2	1.69	0.74
1:C:164:HIS:CD2	1:C:165:PRO:HD2	2.22	0.74
1:C:38:GLU:HB2	1:C:308:THR:HA	1.71	0.72
1:A:194:LYS:HE3	6:A:702:HOH:O	1.89	0.72
1:A:121:GLU:OE1	1:A:344:ARG:NH1	2.23	0.72
1:B:65:LYS:NZ	6:B:683:HOH:O	2.23	0.71
1:B:70:THR:HG23	6:B:573:HOH:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:ASP:HA	1:C:27:HIS:NE2	2.06	0.71
1:A:9:HIS:ND1	1:B:87:PRO:HG2	2.07	0.70
1:B:42:LYS:HG2	1:B:45:LEU:HD21	1.74	0.70
1:D:14:TYR:OH	1:D:19:GLY:HA2	1.92	0.69
1:D:236:LEU:HD12	1:D:236:LEU:H	1.56	0.69
1:B:42:LYS:HD2	1:B:42:LYS:N	2.01	0.69
1:C:26:PRO:O	6:C:871:HOH:O	2.11	0.68
1:C:125:ALA:O	6:C:893:HOH:O	2.11	0.68
1:A:32:PRO:HD3	1:B:79:PHE:CZ	2.29	0.68
1:B:42:LYS:HB2	6:B:613:HOH:O	1.94	0.67
1:C:4:PHE:CD2	1:D:89:ALA:HA	2.29	0.67
1:C:38:GLU:HB2	1:C:308:THR:C	2.20	0.67
1:D:70:THR:HG23	6:D:1184:HOH:O	1.95	0.67
1:D:128:THR:O	1:D:132:LYS:HG3	1.95	0.66
1:A:99:CYS:SG	6:B:557:HOH:O	2.53	0.66
1:A:6:PRO:HB2	6:A:498:HOH:O	1.96	0.66
1:A:177:ASN:ND2	1:B:321:GLU:HB2	2.10	0.66
1:D:5:ASN:N	1:D:9:HIS:ND1	2.43	0.65
1:C:9:HIS:CD2	1:D:87:PRO:HD2	2.29	0.65
1:C:31:ARG:NE	2:D:352:GDU:O2B	2.28	0.65
1:C:243:ARG:NH2	1:C:284:PRO:O	2.26	0.64
1:C:345:GLU:OE1	6:C:1196:HOH:O	2.14	0.64
1:D:94:ASP:OD1	1:D:96:LEU:N	2.27	0.64
1:D:189:TYR:CZ	1:D:193:GLN:HG3	2.33	0.64
1:C:236:LEU:HB2	1:C:237:PRO:HD2	1.80	0.63
1:A:218:HIS:HB2	1:A:254:ASP:OD2	1.98	0.63
1:A:344:ARG:NH2	6:A:572:HOH:O	2.30	0.63
1:B:2:THR:HG22	1:B:3:GLN:N	2.14	0.63
1:B:265:ARG:NH1	1:B:338:VAL:O	2.32	0.62
1:B:342:HIS:HE1	1:B:344:ARG:NH1	1.98	0.62
1:A:98:ARG:HG2	6:A:650:HOH:O	1.99	0.62
1:C:4:PHE:CE1	1:C:6:PRO:HD3	2.34	0.62
1:A:140:GLU:O	1:A:143:LYS:HB2	2.00	0.62
1:C:189:TYR:CE1	1:C:197:MET:HA	2.35	0.62
1:D:43:GLN:HB3	1:D:344:ARG:NH1	2.14	0.61
1:A:94:ASP:O	1:A:98:ARG:HD3	2.00	0.61
1:C:38:GLU:HB2	1:C:308:THR:CA	2.30	0.61
1:D:43:GLN:CB	1:D:344:ARG:NH1	2.63	0.61
1:C:190:PHE:O	1:C:194:LYS:N	2.33	0.61
1:D:162:ASN:OD1	1:D:163:PRO:HD2	2.00	0.61
1:A:62:THR:OG1	1:A:64:ASP:OD2	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLY:O	1:B:113:PRO:HD3	2.01	0.61
1:A:109:ILE:HD12	1:A:133:THR:HG21	1.82	0.60
1:C:48:HIS:CD2	1:C:55:CYS:HB3	2.35	0.60
1:D:119:LEU:HB2	1:D:120:PRO:HD3	1.83	0.60
1:A:65:LYS:HD3	6:A:600:HOH:O	2.01	0.60
1:B:10:PRO:HA	1:B:24:VAL:O	2.01	0.60
1:B:236:LEU:HD23	1:B:236:LEU:N	2.17	0.60
1:B:42:LYS:CD	1:B:45:LEU:HD21	2.32	0.60
1:B:146:PRO:HD2	1:B:172:ASN:O	2.01	0.59
1:C:45:LEU:HB3	1:C:116:SER:HB3	1.85	0.59
1:A:33:TRP:CZ3	1:B:161:SER:HB3	2.37	0.59
1:D:104:GLY:HA2	1:D:145:TYR:CE2	2.38	0.59
1:A:161:SER:O	1:B:34:GLN:HB2	2.01	0.59
1:B:229:TRP:HB2	1:B:232:GLU:HB2	1.85	0.58
1:A:28:ARG:HG2	6:A:569:HOH:O	2.03	0.58
1:C:204:ARG:O	1:C:207:ALA:HB3	2.02	0.58
1:D:43:GLN:NE2	1:D:44:VAL:HG23	2.18	0.58
1:C:45:LEU:HB3	1:C:116:SER:CB	2.34	0.57
1:A:8:ASP:HB3	1:A:27:HIS:HE1	1.69	0.57
1:A:28:ARG:CB	1:A:325:ASP:OD1	2.51	0.57
1:D:49:ASP:O	1:D:51:ASP:N	2.37	0.57
1:B:219:TRP:CZ2	1:B:255:LEU:HB2	2.39	0.57
1:D:203:GLN:HG3	6:D:1205:HOH:O	2.04	0.57
1:B:42:LYS:CG	1:B:45:LEU:HD21	2.34	0.57
1:B:49:ASP:OD1	1:B:50:PRO:HD2	2.05	0.57
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.68	0.57
1:D:43:GLN:CB	1:D:344:ARG:HH12	2.17	0.57
1:A:97:MET:HB3	1:B:225:TYR:CD2	2.40	0.57
1:C:4:PHE:CD1	1:C:4:PHE:C	2.83	0.56
1:D:257:LEU:O	1:D:261:LYS:HG3	2.05	0.56
1:B:89:ALA:HB1	1:B:90:PRO:CD	2.36	0.56
1:A:32:PRO:HG3	1:B:61:VAL:HG21	1.88	0.56
1:C:14:TYR:HB2	1:C:21:TRP:CH2	2.40	0.56
1:C:276:TYR:CD1	1:C:276:TYR:C	2.84	0.56
1:C:4:PHE:HE1	1:C:6:PRO:HG3	1.71	0.56
1:D:190:PHE:O	1:D:194:LYS:N	2.30	0.56
1:C:236:LEU:N	1:C:236:LEU:CD2	2.68	0.56
1:D:326:LEU:HD23	1:D:326:LEU:H	1.71	0.56
1:C:188:GLU:OE2	6:C:1176:HOH:O	2.18	0.55
1:C:280:TRP:CE3	1:C:297:ALA:HB2	2.41	0.55
1:B:343:PHE:CZ	1:B:344:ARG:NH1	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:HIS:HD2	1:D:87:PRO:CD	2.16	0.55
1:D:290:ASN:HA	1:D:292:HIS:CE1	2.41	0.55
1:C:236:LEU:HB2	1:C:237:PRO:CD	2.37	0.55
1:A:14:TYR:OH	1:A:19:GLY:HA2	2.06	0.55
1:A:104:GLY:HA2	1:A:145:TYR:CE1	2.42	0.55
1:B:104:GLY:HA2	1:B:145:TYR:CE1	2.41	0.55
1:D:43:GLN:CD	1:D:44:VAL:HG23	2.32	0.55
1:A:189:TYR:CE1	1:A:197:MET:HA	2.42	0.55
1:C:8:ASP:HA	1:C:27:HIS:HE2	1.72	0.55
1:C:201:TYR:HB2	1:D:96:LEU:HD13	1.89	0.55
1:D:94:ASP:OD2	1:D:95:PRO:HD2	2.06	0.55
1:B:114:ASP:OD1	1:B:116:SER:OG	2.25	0.54
1:D:313:MET:HE2	1:D:322:THR:HG23	1.89	0.54
1:A:14:TYR:CZ	1:A:19:GLY:HA2	2.42	0.54
1:A:28:ARG:HA	6:A:569:HOH:O	2.06	0.54
1:B:2:THR:CG2	1:B:3:GLN:N	2.70	0.54
1:C:114:ASP:OD1	1:C:116:SER:N	2.36	0.54
1:D:98:ARG:NH1	6:D:1172:HOH:O	2.26	0.54
1:D:248:THR:OG1	1:D:251:GLN:HG3	2.07	0.54
1:B:286:ASN:OD1	1:B:288:GLU:HB2	2.08	0.54
1:D:145:TYR:HB3	1:D:172:ASN:O	2.08	0.54
1:A:32:PRO:HD3	1:B:79:PHE:CE1	2.42	0.54
1:D:286:ASN:C	1:D:288:GLU:H	2.16	0.54
1:C:285:PHE:HB3	6:C:1133:HOH:O	2.06	0.54
1:C:26:PRO:HA	1:C:325:ASP:O	2.08	0.54
1:D:88:ASP:HA	1:D:101:SER:OG	2.06	0.54
1:A:41:ALA:HB3	6:A:605:HOH:O	2.08	0.53
1:A:74:VAL:HG22	1:A:109:ILE:HB	1.90	0.53
1:C:321:GLU:HA	6:D:763:HOH:O	2.09	0.53
1:C:104:GLY:HA2	1:C:145:TYR:CE1	2.44	0.53
1:C:323:GLN:NE2	1:C:325:ASP:OD1	2.32	0.53
1:D:212:THR:HA	1:D:222:VAL:HG12	1.90	0.53
1:D:278:MET:HA	1:D:298:HIS:O	2.08	0.53
1:C:321:GLU:HB2	1:D:177:ASN:ND2	2.23	0.53
1:B:219:TRP:CE2	1:B:255:LEU:HB2	2.44	0.53
1:D:161:SER:OG	2:D:352:GDU:H5'2	2.09	0.53
1:D:203:GLN:OE1	1:D:203:GLN:HA	1.98	0.53
1:C:198:LEU:O	1:C:202:VAL:HG23	2.08	0.53
1:D:88:ASP:OD1	1:D:88:ASP:N	2.41	0.53
1:C:9:HIS:CD2	1:D:87:PRO:CG	2.92	0.53
1:B:261:LYS:HE3	6:B:470:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:HIS:CE1	1:B:344:ARG:NH1	2.76	0.53
1:C:22:ILE:HD12	1:C:226:TRP:O	2.09	0.52
1:A:161:SER:HB3	1:B:33:TRP:CZ3	2.45	0.52
1:D:144:THR:HG22	1:D:145:TYR:CE1	2.44	0.52
1:C:38:GLU:N	1:C:308:THR:O	2.34	0.52
1:B:203:GLN:O	1:B:206:LEU:HB2	2.09	0.52
1:C:14:TYR:HB2	1:C:21:TRP:CZ3	2.45	0.52
1:D:38:GLU:HB2	1:D:308:THR:HA	1.92	0.52
1:D:249:ASP:OD1	1:D:252:ARG:NH2	2.42	0.52
1:A:7:VAL:O	1:A:26:PRO:HB3	2.09	0.52
1:C:31:ARG:HD2	2:D:352:GDU:H3D	1.92	0.52
1:C:34:GLN:HE22	1:D:162:ASN:ND2	2.07	0.52
1:C:204:ARG:NH2	1:D:94:ASP:CG	2.68	0.52
1:B:61:VAL:HG11	1:B:79:PHE:CE1	2.44	0.52
1:D:86:THR:O	1:D:103:ARG:HD3	2.10	0.52
1:A:21:TRP:CH2	1:B:100:GLN:HG3	2.45	0.51
1:A:229:TRP:HB2	1:A:232:GLU:HB2	1.92	0.51
1:A:270:PHE:CE1	1:A:306:SER:HA	2.46	0.51
1:A:324:ARG:HH21	1:A:326:LEU:CD2	2.23	0.51
1:B:42:LYS:HD3	1:B:45:LEU:HD21	1.92	0.51
1:B:92:SER:CB	6:B:638:HOH:O	2.51	0.51
1:C:198:LEU:HB2	1:C:294:GLN:HB3	1.91	0.51
1:D:49:ASP:C	1:D:51:ASP:H	2.19	0.51
6:A:398:HOH:O	1:B:10:PRO:HG2	2.10	0.51
1:D:61:VAL:HG12	2:D:352:GDU:C4	2.40	0.51
1:D:120:PRO:O	1:D:260:LYS:NZ	2.43	0.51
1:D:344:ARG:NH2	6:D:1195:HOH:O	2.03	0.51
1:C:36:ALA:HB3	1:C:312:PHE:CZ	2.45	0.51
1:C:112:SER:HB2	1:C:113:PRO:HD2	1.92	0.51
1:D:137:GLN:HB3	1:D:169:ILE:CD1	2.40	0.51
1:D:144:THR:HG22	1:D:145:TYR:CD1	2.46	0.51
1:C:153:ASN:HD21	1:D:315:GLY:CA	2.23	0.51
1:C:204:ARG:NH2	1:D:94:ASP:OD1	2.43	0.51
2:D:352:GDU:O2B	2:D:352:GDU:H3D	2.10	0.51
1:C:48:HIS:NE2	1:C:55:CYS:HB3	2.25	0.51
1:C:190:PHE:CZ	1:C:291:GLN:HG3	2.46	0.51
1:D:314:VAL:HA	1:D:318:MET:HG3	1.91	0.51
1:B:187:LYS:HB3	1:B:187:LYS:HZ2	1.75	0.51
1:C:9:HIS:CD2	1:D:87:PRO:CD	2.92	0.51
1:A:92:SER:OG	1:A:94:ASP:HB2	2.10	0.50
1:B:159:GLY:HA2	6:B:508:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ALA:O	1:D:194:LYS:HE2	2.11	0.50
1:C:40:PRO:HG3	1:C:308:THR:HG22	1.93	0.50
1:C:48:HIS:HD2	6:C:1198:HOH:O	1.94	0.50
1:B:143:LYS:NZ	6:B:483:HOH:O	2.45	0.50
1:D:276:TYR:C	1:D:276:TYR:CD1	2.90	0.50
1:C:154:LYS:CE	1:C:274:PHE:O	2.56	0.50
1:D:49:ASP:C	1:D:51:ASP:N	2.69	0.50
1:D:317:GLU:HA	1:D:321:GLU:O	2.10	0.50
1:A:38:GLU:HB2	1:A:308:THR:HA	1.94	0.49
1:A:172:ASN:ND2	1:A:176:PRO:HG3	2.27	0.49
1:C:342:HIS:HB2	6:C:1196:HOH:O	2.12	0.49
1:D:94:ASP:CG	1:D:95:PRO:HD2	2.37	0.49
1:D:119:LEU:N	1:D:120:PRO:HD2	2.26	0.49
1:B:42:LYS:HG2	1:B:45:LEU:CD2	2.42	0.49
1:B:34:GLN:NE2	6:B:462:HOH:O	2.43	0.49
1:A:9:HIS:CE1	1:B:87:PRO:CG	2.94	0.49
1:A:10:PRO:HA	1:A:24:VAL:O	2.12	0.49
1:C:4:PHE:CD1	1:C:6:PRO:HD3	2.48	0.49
1:C:153:ASN:HD21	1:D:315:GLY:HA3	1.78	0.49
1:D:49:ASP:HB3	1:D:52:CYS:HB2	1.94	0.49
1:B:286:ASN:CG	1:B:288:GLU:HB2	2.38	0.49
1:C:4:PHE:CE2	1:D:89:ALA:HA	2.47	0.49
1:C:114:ASP:OD1	1:C:114:ASP:C	2.55	0.49
1:C:9:HIS:CD2	1:D:87:PRO:HG2	2.48	0.49
1:A:342:HIS:ND1	1:A:344:ARG:HB2	2.28	0.48
1:D:43:GLN:NE2	1:D:44:VAL:CG2	2.76	0.48
1:A:34:GLN:HB2	1:B:161:SER:O	2.13	0.48
1:C:61:VAL:HG11	1:C:79:PHE:HE2	1.79	0.48
1:A:71:GLY:O	1:A:112:SER:HA	2.12	0.48
1:A:319:LEU:HD13	1:B:279:GLY:HA3	1.95	0.48
1:B:335:LEU:O	1:B:338:VAL:HG22	2.12	0.48
1:A:48:HIS:CE1	1:A:55:CYS:HB3	2.48	0.48
1:D:219:TRP:CZ2	1:D:255:LEU:HB2	2.49	0.48
1:A:28:ARG:HB2	1:A:325:ASP:OD1	2.14	0.48
1:C:125:ALA:HB1	6:C:893:HOH:O	2.13	0.48
1:D:144:THR:CG2	1:D:145:TYR:CE1	2.97	0.48
1:C:120:PRO:HB2	1:C:342:HIS:CD2	2.48	0.48
1:D:131:VAL:O	1:D:134:TRP:HB2	2.13	0.47
1:A:79:PHE:CG	1:B:31:ARG:HB3	2.48	0.47
1:C:314:VAL:HA	1:C:318:MET:HG3	1.95	0.47
1:C:2:THR:HB	1:D:87:PRO:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ALA:C	1:C:82:LEU:HG	2.38	0.47
1:C:164:HIS:CD2	1:C:165:PRO:CD	2.97	0.47
1:A:31:ARG:HA	1:B:79:PHE:CE2	2.49	0.47
1:A:2:THR:CG2	1:A:3:GLN:N	2.78	0.47
1:A:145:TYR:HB3	1:A:172:ASN:O	2.15	0.47
1:A:327:THR:HG23	1:A:330:GLN:NE2	2.29	0.47
1:B:317:GLU:HA	1:B:321:GLU:O	2.14	0.47
1:D:23:LEU:O	1:D:323:GLN:HA	2.15	0.47
1:D:98:ARG:HH11	1:D:98:ARG:CG	2.17	0.47
1:D:216:THR:O	1:D:238:LYS:NZ	2.39	0.47
1:D:316:TYR:CD1	1:D:316:TYR:C	2.93	0.47
1:A:69:TYR:CD2	1:A:73:TYR:HB2	2.50	0.47
1:D:119:LEU:HA	1:D:122:LEU:HD12	1.97	0.47
1:D:198:LEU:HB2	1:D:294:GLN:HB3	1.96	0.47
1:A:324:ARG:HH21	1:A:326:LEU:HD23	1.79	0.47
1:D:286:ASN:O	1:D:288:GLU:N	2.48	0.47
1:C:31:ARG:HB2	2:D:352:GDU:O2D	2.14	0.46
1:D:205:GLU:OE1	1:D:211:ARG:NH2	2.40	0.46
1:B:22:ILE:HD12	1:B:22:ILE:N	2.30	0.46
1:B:128:THR:HB	6:B:579:HOH:O	2.15	0.46
1:C:281:HIS:HB2	1:C:296:HIS:CE1	2.50	0.46
1:C:33:TRP:CE3	1:D:161:SER:CB	2.95	0.46
1:C:46:PRO:O	1:C:115:HIS:HB3	2.16	0.46
1:C:73:TYR:CE2	1:C:75:PHE:CD1	3.03	0.46
1:C:240:HIS:NE2	1:C:293:TRP:O	2.46	0.46
1:D:268:ASN:OD1	1:D:343:PHE:HD1	1.98	0.46
1:B:236:LEU:HD23	1:B:236:LEU:H	1.80	0.46
1:B:313:MET:HE2	1:B:322:THR:HG23	1.96	0.46
1:A:5:ASN:O	1:A:8:ASP:N	2.38	0.46
1:B:111:PHE:CD2	1:B:166:GLY:HA2	2.50	0.46
1:C:4:PHE:CE1	1:C:6:PRO:CD	2.98	0.46
1:A:189:TYR:OH	1:A:200:ASP:OD2	2.30	0.46
1:C:161:SER:O	1:D:34:GLN:HB2	2.16	0.46
1:C:168:GLN:C	1:C:169:ILE:HG13	2.41	0.46
1:D:145:TYR:HB3	1:D:146:PRO:HD2	1.98	0.46
1:A:94:ASP:CG	1:B:204:ARG:HH12	2.24	0.46
1:B:21:TRP:C	1:B:22:ILE:HD12	2.40	0.46
1:C:187:LYS:HG2	6:C:1190:HOH:O	2.14	0.46
1:D:271:GLN:OE1	1:D:343:PHE:CG	2.69	0.46
1:D:316:TYR:O	1:D:320:ALA:HB3	2.16	0.46
1:C:320:ALA:HB1	1:D:176:PRO:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:CYS:HB3	1:D:55:CYS:CB	2.41	0.46
1:A:94:ASP:OD2	1:B:204:ARG:NH2	2.48	0.46
2:B:352:GDU:O2B	2:B:352:GDU:H3D	2.16	0.46
1:A:5:ASN:O	1:A:7:VAL:N	2.49	0.45
1:A:278:MET:HA	1:A:298:HIS:O	2.16	0.45
1:C:70:THR:HA	1:C:113:PRO:HG3	1.97	0.45
1:D:112:SER:HB2	1:D:113:PRO:HD2	1.97	0.45
1:D:211:ARG:HD3	1:D:329:GLU:OE2	2.16	0.45
1:A:109:ILE:HD12	1:A:133:THR:CG2	2.46	0.45
1:B:195:SER:OG	1:B:200:ASP:OD1	2.34	0.45
1:B:205:GLU:OE1	1:B:205:GLU:HA	2.16	0.45
1:C:199:VAL:O	1:C:203:GLN:HG2	2.16	0.45
1:D:98:ARG:NH1	1:D:98:ARG:CG	2.78	0.45
1:C:236:LEU:N	1:C:236:LEU:HD23	2.30	0.45
1:D:127:LEU:HD23	1:D:130:ILE:HD12	1.99	0.45
1:D:232:GLU:HG3	1:D:300:TYR:HD1	1.82	0.45
1:A:206:LEU:HD23	1:A:206:LEU:HA	1.79	0.45
1:D:54:LEU:O	1:D:69:TYR:OH	2.34	0.45
1:B:234:LEU:HG	1:B:236:LEU:HD22	1.99	0.45
1:C:280:TRP:CZ3	1:C:297:ALA:HB2	2.52	0.45
1:D:286:ASN:C	1:D:288:GLU:N	2.74	0.45
1:D:211:ARG:HD2	1:D:225:TYR:HA	1.99	0.45
1:A:32:PRO:CD	1:B:79:PHE:CE1	3.00	0.45
1:D:98:ARG:HG2	1:D:98:ARG:NH1	2.09	0.45
1:C:15:ASN:O	1:C:19:GLY:N	2.46	0.44
1:D:44:VAL:O	1:D:44:VAL:HG12	2.17	0.44
1:B:174:PHE:CD1	1:B:174:PHE:N	2.85	0.44
1:D:326:LEU:HD23	1:D:326:LEU:N	2.31	0.44
1:A:96:LEU:HD13	1:B:201:TYR:HA	1.99	0.44
1:A:172:ASN:ND2	1:B:316:TYR:OH	2.50	0.44
1:C:267:ASP:OD2	1:C:342:HIS:NE2	2.29	0.44
1:C:38:GLU:HB2	1:C:308:THR:O	2.18	0.44
1:C:223:VAL:O	1:C:224:PRO:C	2.59	0.44
1:C:228:ALA:HB1	1:C:322:THR:HG21	1.98	0.44
1:A:14:TYR:CE2	1:A:16:PRO:HA	2.52	0.44
1:A:40:PRO:HD3	1:A:308:THR:HG22	1.99	0.44
1:A:176:PRO:CB	1:B:320:ALA:HB1	2.48	0.44
1:C:212:THR:HA	1:C:222:VAL:HG12	1.99	0.44
1:A:69:TYR:CG	1:A:73:TYR:HB2	2.53	0.44
1:A:5:ASN:C	1:A:7:VAL:N	2.76	0.43
1:A:177:ASN:HD22	1:B:321:GLU:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:HIS:CE1	1:A:344:ARG:HB2	2.53	0.43
1:B:268:ASN:OD1	1:B:343:PHE:HD1	2.00	0.43
1:C:40:PRO:HD3	1:C:308:THR:HG22	1.99	0.43
1:C:281:HIS:CB	1:C:296:HIS:CE1	3.01	0.43
1:C:227:ALA:HB1	1:C:232:GLU:HB3	1.99	0.43
1:D:53:PHE:HD1	1:D:60:ARG:HA	1.83	0.43
1:D:313:MET:HE2	6:D:1113:HOH:O	2.17	0.43
1:D:82:LEU:CD1	1:D:172:ASN:HD22	2.31	0.43
1:A:3:GLN:HA	1:A:3:GLN:NE2	2.24	0.43
1:A:38:GLU:CB	1:A:308:THR:HA	2.49	0.43
1:A:140:GLU:HA	1:A:143:LYS:NZ	2.34	0.43
1:A:163:PRO:HG2	6:A:687:HOH:O	2.19	0.43
1:C:22:ILE:HD11	6:C:805:HOH:O	2.18	0.43
1:D:208:ASP:OD1	1:D:210:SER:OG	2.31	0.43
1:C:7:VAL:O	1:C:26:PRO:HB2	2.18	0.43
1:D:26:PRO:HD2	6:D:772:HOH:O	2.18	0.43
1:C:37:GLN:HG3	1:C:308:THR:HB	2.01	0.43
1:D:229:TRP:HB2	1:D:232:GLU:HB2	2.00	0.43
1:D:243:ARG:NH2	1:D:284:PRO:O	2.33	0.43
1:D:303:LEU:HD13	1:D:307:ALA:HA	1.99	0.43
1:A:49:ASP:OD1	1:A:50:PRO:HD2	2.19	0.43
1:D:76:THR:O	1:D:77:ASN:C	2.58	0.43
1:D:119:LEU:N	1:D:120:PRO:CD	2.81	0.43
1:D:268:ASN:O	1:D:271:GLN:NE2	2.51	0.43
1:A:70:THR:HA	1:A:113:PRO:HG3	2.00	0.43
1:B:2:THR:CG2	1:B:3:GLN:H	2.29	0.43
1:A:25:SER:HA	1:A:26:PRO:HD2	1.71	0.43
1:B:290:ASN:HA	1:B:292:HIS:CE1	2.54	0.43
1:C:190:PHE:CD1	1:C:190:PHE:C	2.97	0.43
1:C:4:PHE:HB2	1:D:88:ASP:O	2.19	0.42
1:A:320:ALA:HB1	1:B:176:PRO:CB	2.49	0.42
1:B:344:ARG:NH2	6:B:646:HOH:O	2.51	0.42
1:C:278:MET:SD	1:C:278:MET:C	3.01	0.42
1:D:53:PHE:O	1:D:66:ASN:ND2	2.47	0.42
1:A:25:SER:OG	1:B:81:ALA:O	2.33	0.42
1:A:89:ALA:O	1:A:91:GLU:HG3	2.19	0.42
1:A:276:TYR:CD1	1:A:276:TYR:C	2.97	0.42
1:C:324:ARG:HH11	1:C:324:ARG:HD2	1.62	0.42
1:B:57:GLY:HA2	1:B:66:ASN:O	2.20	0.42
1:B:342:HIS:O	1:B:344:ARG:N	2.53	0.42
1:B:212:THR:HA	1:B:222:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ALA:O	1:B:241:VAL:HG23	2.19	0.42
1:D:88:ASP:HA	1:D:101:SER:HG	1.84	0.42
1:D:324:ARG:NE	1:D:326:LEU:O	2.44	0.42
1:A:104:GLY:HA2	1:A:145:TYR:CZ	2.54	0.42
1:A:189:TYR:CZ	1:A:193:GLN:HG3	2.54	0.42
1:D:169:ILE:HG21	1:D:169:ILE:HD13	1.80	0.42
1:D:209:GLY:HA2	6:D:867:HOH:O	2.19	0.42
1:D:221:ALA:HB2	1:D:235:LEU:HD13	2.02	0.42
1:A:83:MET:HE1	6:A:615:HOH:O	2.19	0.42
1:D:189:TYR:CD1	1:D:189:TYR:C	2.98	0.42
1:B:43:GLN:OE1	1:B:344:ARG:HD3	2.19	0.42
1:C:117:LYS:HD3	1:C:122:LEU:HD23	2.02	0.42
1:D:48:HIS:HE1	1:D:50:PRO:HA	1.84	0.42
1:D:218:HIS:HB2	1:D:219:TRP:CD1	2.55	0.42
1:A:289:GLU:HG3	6:A:496:HOH:O	2.20	0.41
1:C:41:ALA:HA	6:C:1075:HOH:O	2.19	0.41
1:D:55:CYS:HB2	1:D:58:ASN:ND2	2.35	0.41
1:D:247:LEU:HA	1:D:251:GLN:OE1	2.19	0.41
1:A:99:CYS:HB3	1:B:225:TYR:OH	2.19	0.41
1:B:120:PRO:HB3	1:B:263:THR:OG1	2.20	0.41
1:D:176:PRO:O	1:D:177:ASN:C	2.64	0.41
1:D:18:THR:HA	1:D:181:ARG:HD2	2.02	0.41
1:D:174:PHE:CD1	1:D:174:PHE:N	2.88	0.41
1:A:15:ASN:C	1:A:15:ASN:OD1	2.63	0.41
1:B:120:PRO:O	1:B:260:LYS:NZ	2.54	0.41
1:B:288:GLU:HG3	6:B:612:HOH:O	2.20	0.41
1:C:4:PHE:CE2	1:D:89:ALA:HB2	2.55	0.41
1:C:201:TYR:CE1	1:D:97:MET:HE2	2.56	0.41
1:D:146:PRO:HD2	1:D:172:ASN:O	2.21	0.41
1:D:232:GLU:HG3	1:D:299:PHE:O	2.20	0.41
1:B:69:TYR:CG	1:B:73:TYR:HB2	2.55	0.41
1:B:96:LEU:C	1:B:97:MET:HG3	2.46	0.41
1:C:31:ARG:HG2	1:C:31:ARG:NH1	2.32	0.41
1:C:112:SER:CB	1:C:113:PRO:HD2	2.50	0.41
1:D:228:ALA:HB1	1:D:322:THR:HG21	2.03	0.41
1:A:97:MET:HB3	1:B:225:TYR:CE2	2.56	0.41
1:B:162:ASN:HA	1:B:163:PRO:HD3	1.85	0.41
1:B:236:LEU:N	1:B:236:LEU:CD2	2.83	0.41
1:B:303:LEU:HD23	1:B:303:LEU:HA	1.79	0.41
1:C:146:PRO:HD2	1:C:173:SER:HA	2.03	0.41
1:D:152:GLU:HB3	1:D:278:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:THR:HG22	1:A:3:GLN:N	2.35	0.41
1:B:211:ARG:HH11	1:B:211:ARG:HD3	1.69	0.41
1:C:45:LEU:HB3	1:C:116:SER:HB2	2.03	0.41
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.77	0.41
1:D:257:LEU:HD11	1:D:261:LYS:HE2	2.02	0.41
1:A:28:ARG:HB3	1:A:325:ASP:OD1	2.20	0.40
1:A:213:VAL:HG12	1:A:214:VAL:HG23	2.02	0.40
1:A:174:PHE:CD1	1:A:174:PHE:N	2.88	0.40
1:A:324:ARG:NH2	1:A:326:LEU:HD21	2.36	0.40
1:C:18:THR:HB	1:C:181:ARG:CZ	2.52	0.40
1:C:162:ASN:OD1	1:C:163:PRO:HD2	2.22	0.40
1:D:31:ARG:HB2	1:D:32:PRO:HD2	2.03	0.40
1:D:137:GLN:HB3	1:D:169:ILE:HD13	2.01	0.40
1:A:326:LEU:HD23	1:A:326:LEU:C	2.46	0.40
1:C:49:ASP:HA	1:C:50:PRO:HD2	1.85	0.40
1:A:299:PHE:O	1:A:301:PRO:HD3	2.21	0.40
1:B:189:TYR:CG	1:B:197:MET:HB2	2.56	0.40
1:B:206:LEU:HA	1:B:206:LEU:HD23	1.71	0.40
1:C:27:HIS:C	1:C:29:ALA:N	2.79	0.40
1:D:189:TYR:CE1	1:D:197:MET:HA	2.56	0.40
1:A:319:LEU:CD1	1:B:279:GLY:HA3	2.51	0.40
1:B:67:PRO:HA	6:B:683:HOH:O	2.21	0.40
1:D:4:PHE:HA	1:D:9:HIS:ND1	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1190:HOH:O	6:C:1239:HOH:O[2_657]	1.72	0.48

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	345/348 (99%)	325 (94%)	18 (5%)	2 (1%)	21	11
1	B	342/348 (98%)	325 (95%)	16 (5%)	1 (0%)	36	25
1	C	342/348 (98%)	321 (94%)	19 (6%)	2 (1%)	21	11
1	D	342/348 (98%)	324 (95%)	16 (5%)	2 (1%)	21	11
All	All	1371/1392 (98%)	1295 (94%)	69 (5%)	7 (0%)	24	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	43	GLN
1	C	44	VAL
1	A	26	PRO
1	B	343	PHE
1	D	50	PRO
1	D	287	GLY
1	A	6	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	297/298 (100%)	279 (94%)	18 (6%)	17	6
1	B	295/298 (99%)	277 (94%)	18 (6%)	17	6
1	C	295/298 (99%)	276 (94%)	19 (6%)	16	6
1	D	295/298 (99%)	276 (94%)	19 (6%)	16	6
All	All	1182/1192 (99%)	1108 (94%)	74 (6%)	16	6

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	7	VAL
1	A	8	ASP
1	A	22	ILE

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Mol	Chain	Res	Type
1	A	38	GLU
1	A	42	LYS
1	A	43	GLN
1	A	44	VAL
1	A	83	MET
1	A	109	ILE
1	A	123	SER
1	A	124	VAL
1	A	143	LYS
1	A	194	LYS
1	A	236	LEU
1	A	253	SER
1	A	288	GLU
1	A	326	LEU
1	B	3	GLN
1	B	8	ASP
1	B	22	ILE
1	B	42	LYS
1	B	44	VAL
1	B	91	GLU
1	B	92	SER
1	B	109	ILE
1	B	112	SER
1	B	187	LYS
1	B	194	LYS
1	B	197	MET
1	B	202	VAL
1	B	211	ARG
1	B	253	SER
1	B	288	GLU
1	B	289	GLU
1	B	321	GLU
1	C	2	THR
1	C	3	GLN
1	C	7	VAL
1	C	22	ILE
1	C	30	LYS
1	C	31	ARG
1	C	37	GLN
1	C	39	THR
1	C	42	LYS
1	C	45	LEU

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Mol	Chain	Res	Type
1	C	109	ILE
1	C	194	LYS
1	C	204	ARG
1	C	236	LEU
1	C	242	LEU
1	C	245	THR
1	C	253	SER
1	C	266	TYR
1	C	313	MET
1	D	43	GLN
1	D	59	VAL
1	D	88	ASP
1	D	91	GLU
1	D	98	ARG
1	D	99	CYS
1	D	101	SER
1	D	119	LEU
1	D	129	GLU
1	D	136	GLU
1	D	195	SER
1	D	203	GLN
1	D	236	LEU
1	D	242	LEU
1	D	253	SER
1	D	262	LEU
1	D	266	TYR
1	D	288	GLU
1	D	289	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	20	GLN
1	A	27	HIS
1	A	34	GLN
1	A	37	GLN
1	A	93	HIS
1	A	100	GLN
1	A	172	ASN
1	A	193	GLN
1	A	330	GLN

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Mol	Chain	Res	Type
1	B	37	GLN
1	B	291	GLN
1	C	3	GLN
1	C	34	GLN
1	C	37	GLN
1	C	48	HIS
1	C	100	GLN
1	C	153	ASN
1	C	172	ASN
1	C	193	GLN
1	C	271	GLN
1	D	37	GLN
1	D	43	GLN
1	D	48	HIS
1	D	100	GLN
1	D	193	GLN
1	D	291	GLN

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 16 ligands modelled in this entry, 12 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
2	GDU	A	352	-	37,38,38	1.12	1 (2%)	55,58,58	1.09	2 (3%)
2	GDU	D	352	-	37,38,38	1.43	1 (2%)	55,58,58	1.16	5 (9%)
2	GDU	C	352	-	37,38,38	1.41	3 (8%)	55,58,58	1.32	7 (12%)
2	GDU	B	352	-	37,38,38	1.26	2 (5%)	55,58,58	1.10	3 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDU	A	352	-	-	8/23/59/59	0/3/3/3
2	GDU	D	352	-	-	7/23/59/59	0/3/3/3
2	GDU	C	352	-	-	7/23/59/59	0/3/3/3
2	GDU	B	352	-	-	8/23/59/59	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	352	GDU	PA-O3A	7.40	1.67	1.59
2	C	352	GDU	PB-O3A	-4.95	1.54	1.59
2	A	352	GDU	PA-O3A	4.84	1.64	1.59
2	B	352	GDU	PA-O3A	4.45	1.64	1.59
2	C	352	GDU	PA-O3A	4.24	1.64	1.59
2	B	352	GDU	PB-O3A	-3.78	1.55	1.59
2	C	352	GDU	O4-C4	-2.36	1.19	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	352	GDU	C1'-O5'-C5'	3.68	120.90	113.72
2	C	352	GDU	O3A-PB-O1B	3.35	120.77	110.70
2	C	352	GDU	O5'-C1'-O3B	-3.05	107.38	111.36
2	D	352	GDU	O5'-C5'-C4'	2.72	114.60	109.70
2	B	352	GDU	O4'-C4'-C5'	2.67	115.89	109.32
2	C	352	GDU	C4D-O4D-C1D	-2.60	103.72	109.47
2	B	352	GDU	O4D-C4D-C3D	2.50	110.11	105.15
2	C	352	GDU	C4-N3-C2	-2.49	123.52	126.61
2	D	352	GDU	O2B-PB-O3A	2.48	113.97	107.27
2	C	352	GDU	O5D-PA-O1A	2.40	118.45	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	352	GDU	O3'-C3'-C2'	-2.33	104.89	110.38
2	B	352	GDU	O5'-C5'-C4'	2.23	113.71	109.70
2	C	352	GDU	O4D-C4D-C3D	2.21	109.55	105.15
2	A	352	GDU	O4D-C4D-C3D	2.20	109.52	105.15
2	D	352	GDU	C4'-C3'-C2'	-2.12	107.10	110.83
2	D	352	GDU	O4-C4-C5	2.05	128.69	125.16
2	C	352	GDU	C3'-C4'-C5'	-2.03	106.56	110.23

There are no chirality outliers.

All (30) torsion outliers are listed below:

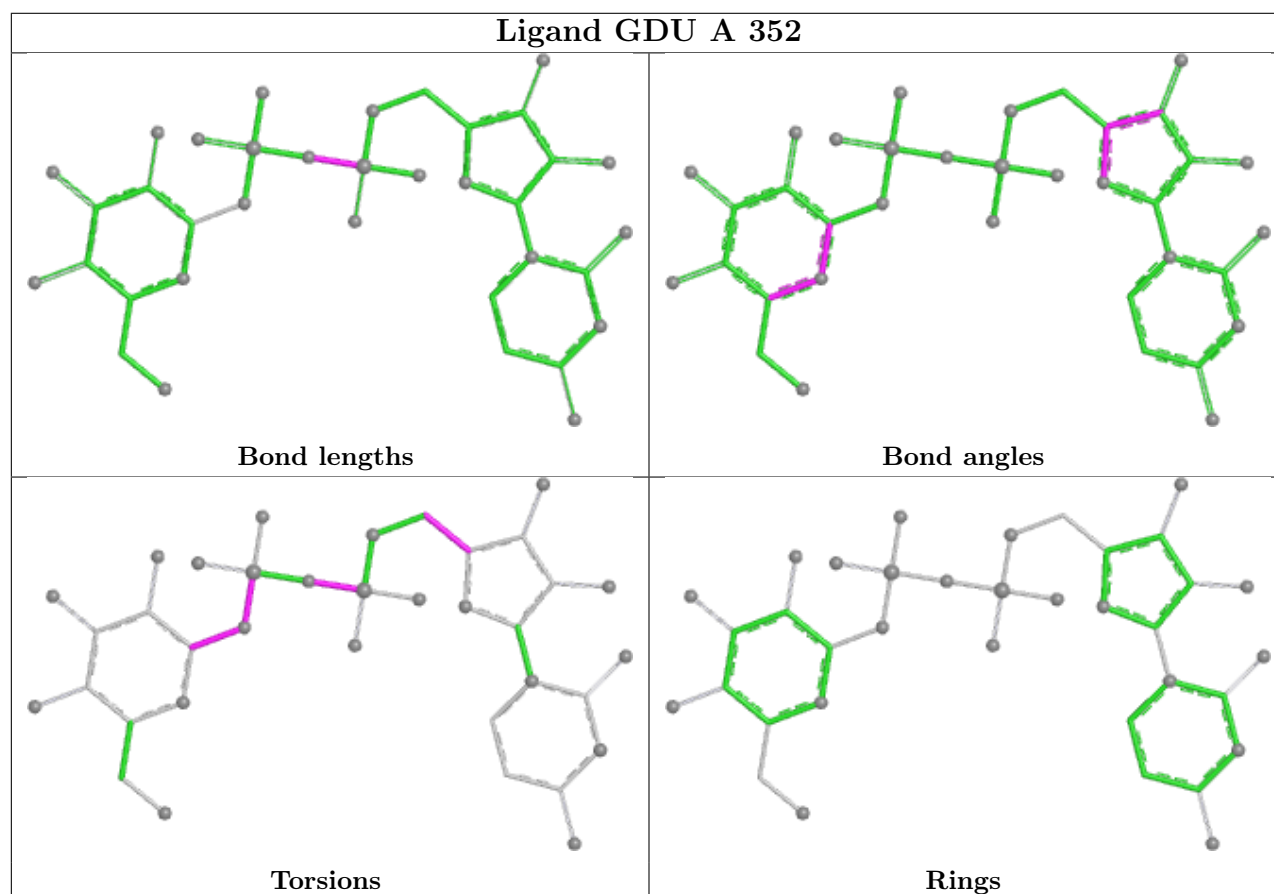
Mol	Chain	Res	Type	Atoms
2	A	352	GDU	PB-O3A-PA-O5D
2	A	352	GDU	C1'-O3B-PB-O3A
2	B	352	GDU	PB-O3A-PA-O5D
2	B	352	GDU	C1'-O3B-PB-O3A
2	C	352	GDU	C5D-O5D-PA-O2A
2	C	352	GDU	C5D-O5D-PA-O3A
2	C	352	GDU	C1'-O3B-PB-O3A
2	D	352	GDU	C1'-O3B-PB-O3A
2	D	352	GDU	O4D-C4D-C5D-O5D
2	A	352	GDU	O4D-C4D-C5D-O5D
2	D	352	GDU	C3D-C4D-C5D-O5D
2	B	352	GDU	O4D-C4D-C5D-O5D
2	B	352	GDU	C2'-C1'-O3B-PB
2	C	352	GDU	C2'-C1'-O3B-PB
2	B	352	GDU	C3D-C4D-C5D-O5D
2	C	352	GDU	PB-O3A-PA-O1A
2	D	352	GDU	PB-O3A-PA-O1A
2	A	352	GDU	C3D-C4D-C5D-O5D
2	C	352	GDU	PB-O3A-PA-O5D
2	D	352	GDU	PB-O3A-PA-O5D
2	C	352	GDU	C1'-O3B-PB-O1B
2	D	352	GDU	C1'-O3B-PB-O1B
2	A	352	GDU	C2'-C1'-O3B-PB
2	D	352	GDU	C2'-C1'-O3B-PB
2	A	352	GDU	C1'-O3B-PB-O1B
2	B	352	GDU	C1'-O3B-PB-O1B
2	A	352	GDU	PB-O3A-PA-O1A
2	A	352	GDU	PB-O3A-PA-O2A
2	B	352	GDU	PB-O3A-PA-O1A
2	B	352	GDU	PB-O3A-PA-O2A

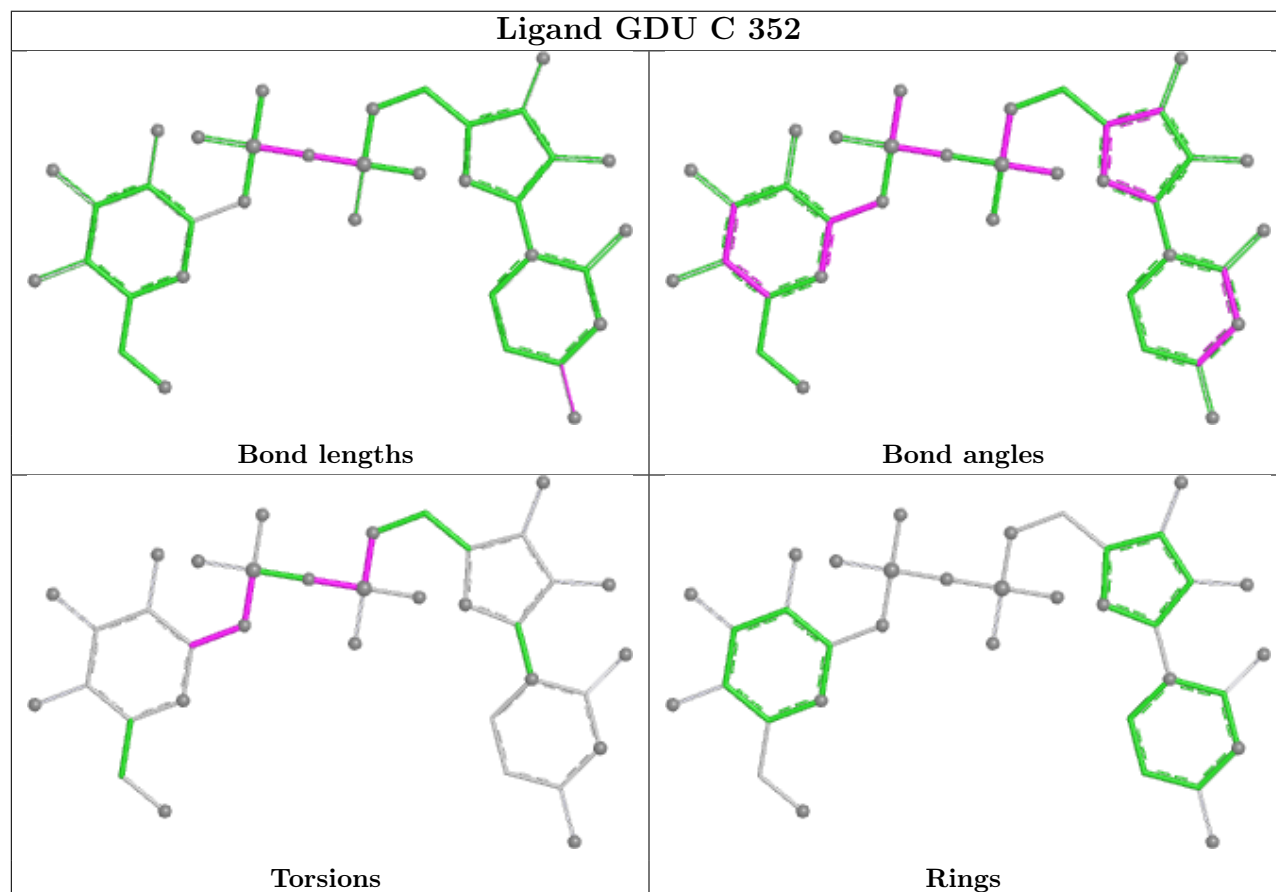
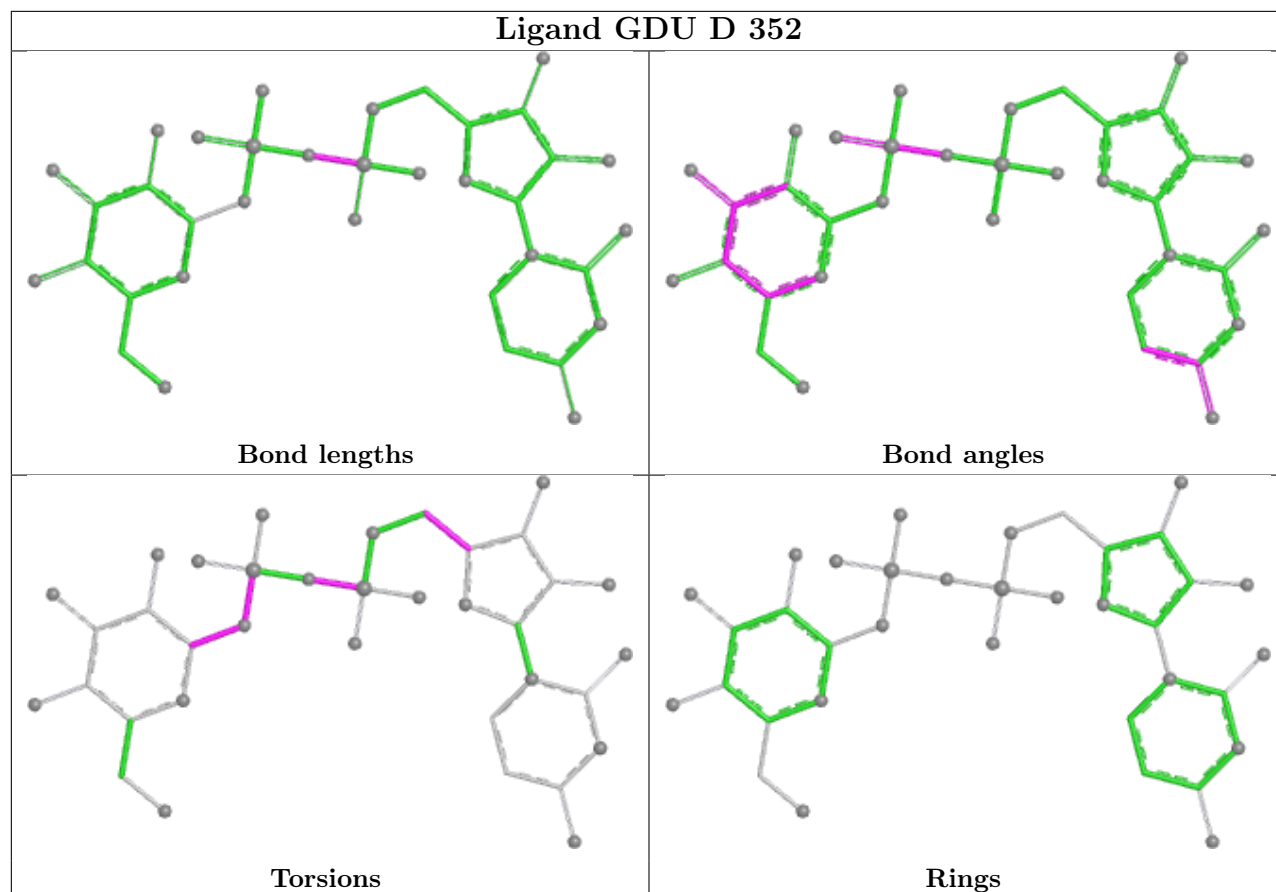
There are no ring outliers.

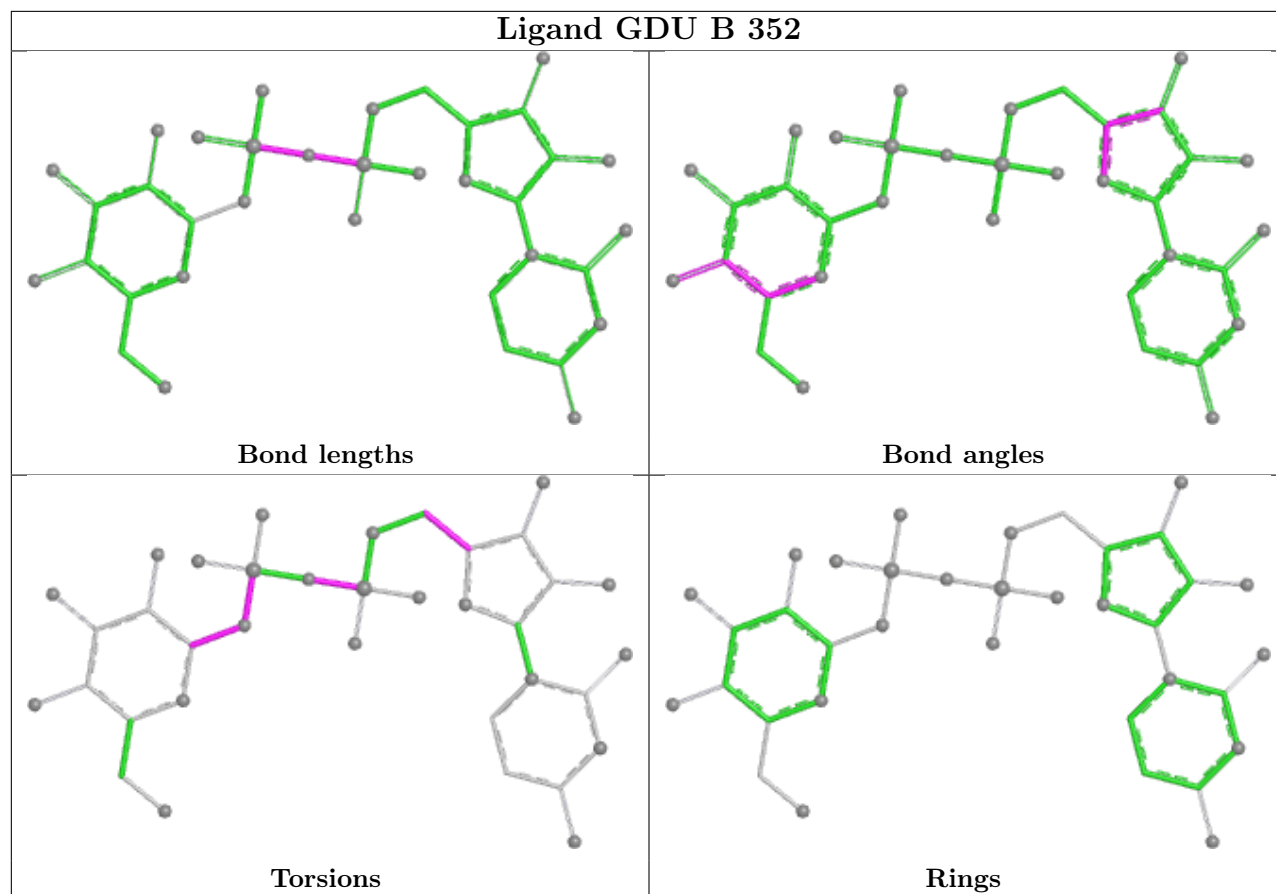
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	352	GDU	7	0
2	B	352	GDU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.