



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:44 PM UTC

PDB ID : 1DE6 / pdb_00001de6
Title : L-RHAMNOSE ISOMERASE
Authors : Korndorfer, I.P.; Fessner, W.D.; Matthews, B.W.
Deposited on : 1999-11-13
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

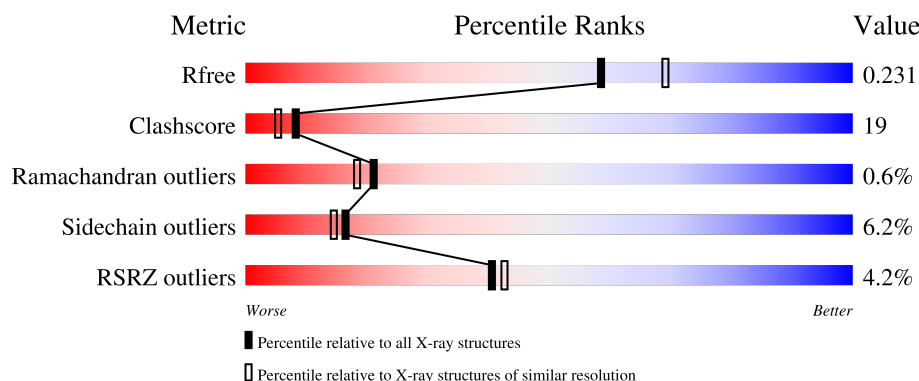
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

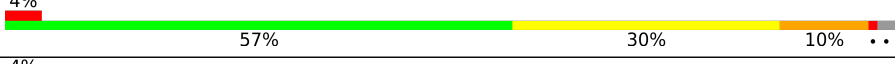
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	426	
1	B	426	
1	C	426	
1	D	426	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14331 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 L-RHAMNOSE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3309	2090	587	619	13			
1	B	416	Total	C	N	O	S	0	0	0
			3309	2090	587	619	13			
1	C	416	Total	C	N	O	S	0	0	0
			3309	2090	587	619	13			
1	D	416	Total	C	N	O	S	0	0	0
			3309	2090	587	619	13			

There are 28 discrepancies between the modelled and reference sequences:

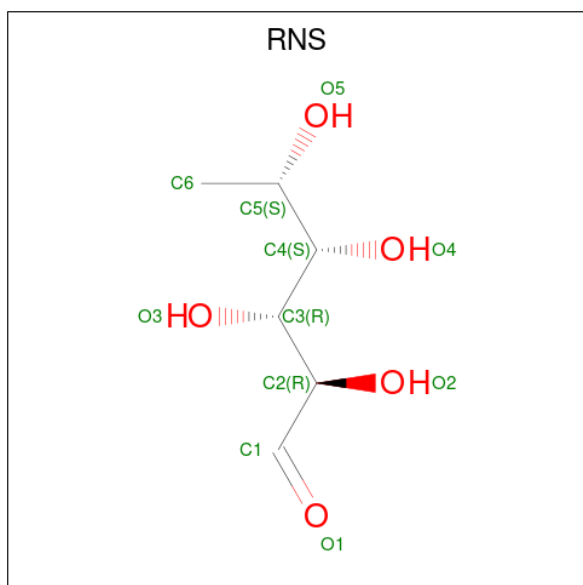
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	expression tag	UNP P32170
A	3	HIS	-	expression tag	UNP P32170
A	4	HIS	-	expression tag	UNP P32170
A	5	HIS	-	expression tag	UNP P32170
A	6	HIS	-	expression tag	UNP P32170
A	7	HIS	-	expression tag	UNP P32170
A	8	HIS	-	expression tag	UNP P32170
B	2	GLY	-	expression tag	UNP P32170
B	3	HIS	-	expression tag	UNP P32170
B	4	HIS	-	expression tag	UNP P32170
B	5	HIS	-	expression tag	UNP P32170
B	6	HIS	-	expression tag	UNP P32170
B	7	HIS	-	expression tag	UNP P32170
B	8	HIS	-	expression tag	UNP P32170
C	2	GLY	-	expression tag	UNP P32170
C	3	HIS	-	expression tag	UNP P32170
C	4	HIS	-	expression tag	UNP P32170
C	5	HIS	-	expression tag	UNP P32170
C	6	HIS	-	expression tag	UNP P32170
C	7	HIS	-	expression tag	UNP P32170
C	8	HIS	-	expression tag	UNP P32170

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	GLY	-	expression tag	UNP P32170
D	3	HIS	-	expression tag	UNP P32170
D	4	HIS	-	expression tag	UNP P32170
D	5	HIS	-	expression tag	UNP P32170
D	6	HIS	-	expression tag	UNP P32170
D	7	HIS	-	expression tag	UNP P32170
D	8	HIS	-	expression tag	UNP P32170

- Molecule 2 is L-RHAMNOSE (CCD ID: RNS) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	C	1	Total	C	O	0	0
			11	6	5		
2	D	1	Total	C	O	0	0
			11	6	5		

- 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		

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

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

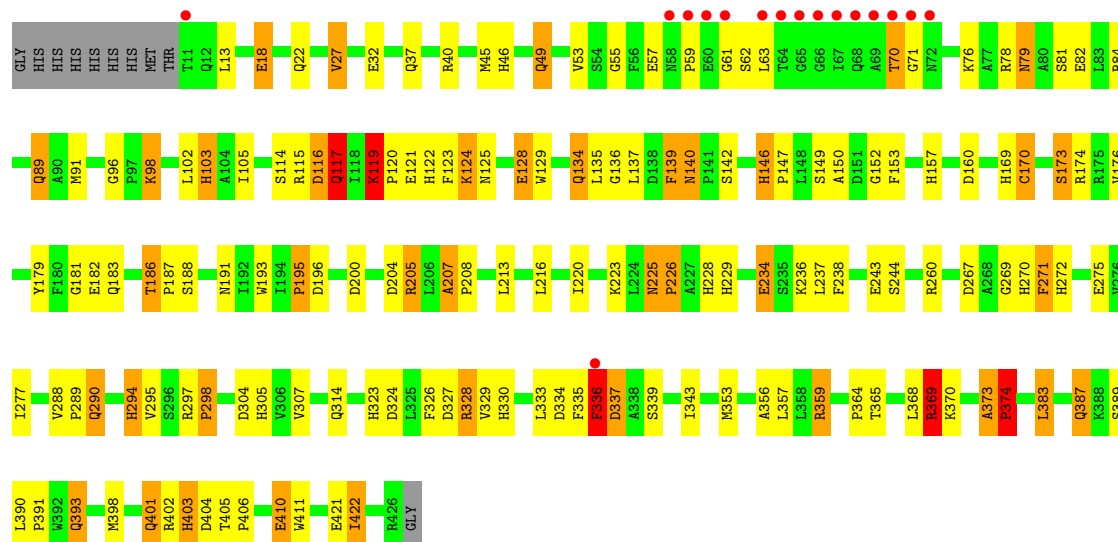
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mn 1	0	0
4	B	1	Total 1	Mn 1	0	0
4	C	1	Total 1	Mn 1	0	0
4	D	1	Total 1	Mn 1	0	0

- Molecule 5 is water.

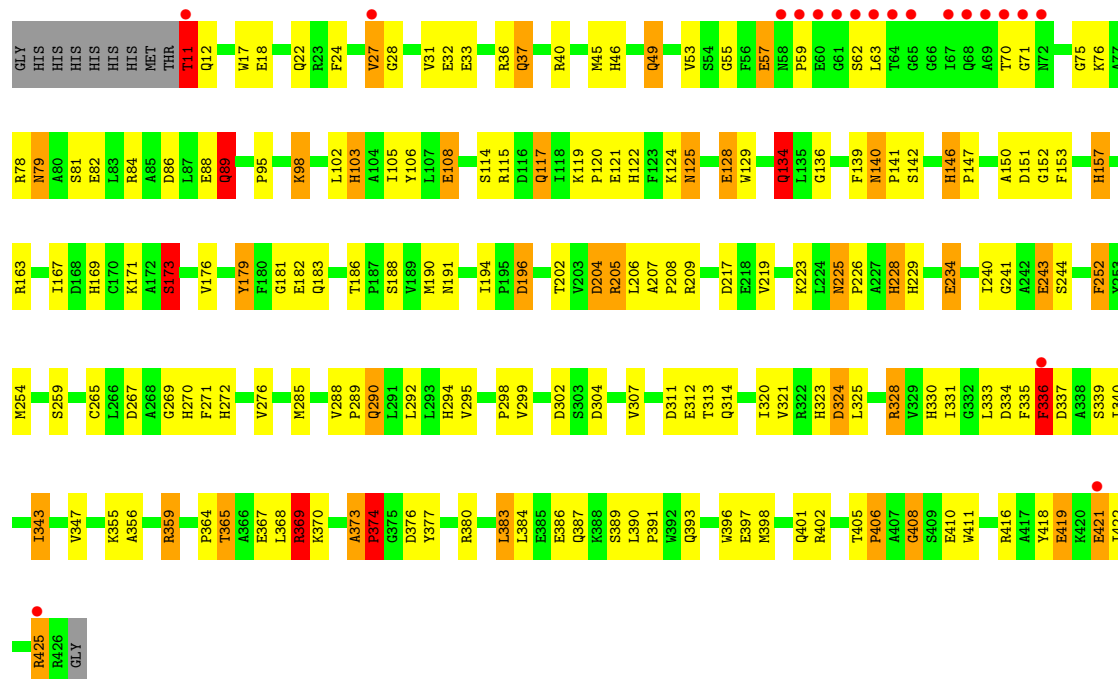
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	250	Total 250	O 250	0	0
5	B	286	Total 286	O 286	0	0
5	C	263	Total 263	O 263	0	0
5	D	244	Total 244	O 244	0	0



• Molecule 1: L-RHAMNOSE ISOMERASE



• Molecule 1: L-RHAMNOSE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.18Å 162.44Å 77.73Å 90.00° 109.89° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	87.0 (30.00-2.10) 92.2 (30.00-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.10Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.244 , 0.244 0.172 , 0.231	Depositor DCC
R_{free} test set	5391 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 112.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14331	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: RNS, MN, 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	1.58	21/3389 (0.6%)	1.92	79/4602 (1.7%)
1	B	1.60	22/3389 (0.6%)	1.96	79/4602 (1.7%)
1	C	1.57	16/3389 (0.5%)	1.93	71/4602 (1.5%)
1	D	1.55	13/3389 (0.4%)	1.94	90/4602 (2.0%)
All	All	1.58	72/13556 (0.5%)	1.94	319/18408 (1.7%)

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	374	PRO	CA-C	-8.95	1.43	1.52
1	B	272	HIS	ND1-CE1	8.53	1.41	1.32
1	A	272	HIS	ND1-CE1	8.26	1.40	1.32
1	B	374	PRO	CA-C	-8.23	1.44	1.52
1	C	272	HIS	ND1-CE1	7.85	1.40	1.32
1	D	272	HIS	ND1-CE1	7.68	1.40	1.32
1	B	374	PRO	N-CA	-7.38	1.41	1.47
1	C	146	HIS	ND1-CE1	6.95	1.39	1.32
1	D	311	ASP	C-O	-6.88	1.16	1.24
1	C	191	ASN	CA-C	-6.88	1.44	1.52
1	B	334	ASP	CG-OD2	6.87	1.38	1.25
1	A	32	GLU	CD-OE2	6.58	1.37	1.25
1	A	138	ASP	CG-OD2	6.49	1.37	1.25
1	B	272	HIS	CG-CD2	6.43	1.43	1.35
1	C	298	PRO	CA-C	6.26	1.59	1.52
1	B	359	ARG	CZ-NH1	6.14	1.41	1.32
1	A	146	HIS	ND1-CE1	5.93	1.38	1.32
1	A	374	PRO	CA-C	-5.81	1.46	1.52
1	C	146	HIS	CG-CD2	5.80	1.42	1.35
1	D	146	HIS	ND1-CE1	5.77	1.38	1.32
1	D	359	ARG	CZ-NH1	5.76	1.40	1.32
1	C	229	HIS	ND1-CE1	5.72	1.38	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ARG	NE-CZ	5.66	1.39	1.33
1	A	41	LEU	C-O	-5.61	1.18	1.24
1	D	36	ARG	C-N	-5.61	1.26	1.33
1	D	108	GLU	CD-OE2	5.58	1.35	1.25
1	A	273	PRO	N-CA	-5.54	1.40	1.47
1	D	347	VAL	N-CA	-5.51	1.40	1.46
1	D	376	ASP	CA-C	5.49	1.59	1.53
1	A	272	HIS	CG-CD2	5.46	1.41	1.35
1	C	140	ASN	CG-OD1	5.44	1.33	1.23
1	B	218	GLU	CD-OE2	5.42	1.35	1.25
1	A	27	VAL	CA-C	-5.41	1.45	1.52
1	B	146	HIS	CG-CD2	5.40	1.41	1.35
1	C	18	GLU	CD-OE2	5.38	1.35	1.25
1	B	391	PRO	N-CA	-5.37	1.43	1.47
1	B	146	HIS	ND1-CE1	5.36	1.38	1.32
1	A	289	PRO	C-N	-5.36	1.27	1.33
1	B	422	ILE	N-CA	-5.35	1.41	1.46
1	D	397	GLU	CD-OE2	5.34	1.35	1.25
1	B	31	VAL	N-CA	-5.33	1.39	1.46
1	D	259	SER	N-CA	-5.33	1.39	1.46
1	C	403	HIS	CD2-NE2	5.29	1.43	1.37
1	B	342	ARG	C-O	-5.29	1.17	1.24
1	C	103	HIS	CG-CD2	5.28	1.41	1.35
1	A	391	PRO	N-CD	5.27	1.55	1.47
1	A	204	ASP	C-O	-5.27	1.18	1.24
1	C	183	GLN	CA-C	-5.27	1.46	1.52
1	A	142	SER	CA-C	-5.27	1.46	1.53
1	B	279	ASP	CG-OD2	5.26	1.35	1.25
1	A	229	HIS	CG-CD2	5.26	1.41	1.35
1	D	321	VAL	N-CA	-5.24	1.40	1.46
1	B	128	GLU	CD-OE2	5.23	1.35	1.25
1	A	142	SER	C-O	-5.22	1.17	1.23
1	B	319	GLU	CD-OE2	5.21	1.35	1.25
1	A	164	GLN	C-N	-5.19	1.27	1.33
1	B	83	LEU	N-CA	-5.18	1.40	1.46
1	A	311	ASP	CG-OD2	5.18	1.35	1.25
1	D	323	HIS	CG-ND1	5.18	1.44	1.38
1	B	94	ILE	N-CA	-5.17	1.41	1.46
1	C	176	VAL	CA-CB	-5.16	1.48	1.54
1	C	32	GLU	CD-OE2	5.16	1.35	1.25
1	B	176	VAL	CA-C	5.14	1.59	1.52
1	C	170	CYS	C-O	5.13	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	GLY	N-CA	5.11	1.50	1.45
1	B	302	ASP	CG-OD2	5.07	1.34	1.25
1	B	17	TRP	NE1-CE2	-5.06	1.31	1.37
1	A	217	ASP	CG-OD2	5.05	1.34	1.25
1	A	36	ARG	CZ-NH1	5.05	1.39	1.32
1	B	416	ARG	N-CA	-5.04	1.40	1.46
1	D	421	GLU	CD-OE2	5.01	1.34	1.25
1	C	334	ASP	CG-OD2	5.01	1.34	1.25

All (319) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	205	ARG	NE-CZ-NH2	-13.03	107.48	119.20
1	C	374	PRO	CA-N-CD	-9.96	98.06	112.00
1	B	359	ARG	NE-CZ-NH2	-9.67	110.50	119.20
1	C	294	HIS	CA-CB-CG	-9.53	104.27	113.80
1	B	272	HIS	CB-CG-CD2	-9.27	119.15	131.20
1	B	324	ASP	CA-CB-CG	-9.24	103.36	112.60
1	A	374	PRO	CA-N-CD	-9.18	99.15	112.00
1	B	27	VAL	CA-C-O	9.08	128.90	119.91
1	C	373	ALA	C-N-CD	-9.01	88.08	125.00
1	C	359	ARG	NE-CZ-NH2	-8.98	111.12	119.20
1	C	422	ILE	N-CA-C	8.89	119.84	111.48
1	B	373	ALA	C-N-CD	-8.88	88.58	125.00
1	C	205	ARG	NE-CZ-NH1	8.86	130.36	121.50
1	B	252	PHE	CA-CB-CG	-8.61	105.19	113.80
1	A	205	ARG	CD-NE-CZ	8.49	136.29	124.40
1	D	374	PRO	CA-N-CD	-8.49	100.11	112.00
1	D	146	HIS	CB-CG-CD2	-8.49	120.17	131.20
1	B	374	PRO	CA-N-CD	-8.38	100.27	112.00
1	D	271	PHE	CA-CB-CG	-8.36	105.44	113.80
1	A	373	ALA	C-N-CD	-8.29	90.99	125.00
1	D	205	ARG	NE-CZ-NH1	8.28	129.78	121.50
1	C	57	GLU	CA-C-N	8.27	130.06	122.37
1	C	57	GLU	C-N-CA	8.27	130.06	122.37
1	C	205	ARG	CD-NE-CZ	8.26	135.97	124.40
1	D	270	HIS	N-CA-C	8.21	122.08	112.72
1	C	270	HIS	N-CA-C	8.21	123.01	112.92
1	A	146	HIS	CB-CG-CD2	-8.17	120.58	131.20
1	C	272	HIS	CB-CG-CD2	-8.16	120.59	131.20
1	A	187	PRO	N-CA-CB	8.13	110.41	103.25
1	D	373	ALA	C-N-CD	-8.00	92.21	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	271	PHE	CA-CB-CG	-7.98	105.82	113.80
1	A	205	ARG	NE-CZ-NH1	7.97	129.47	121.50
1	B	146	HIS	CB-CG-CD2	-7.88	120.96	131.20
1	B	117	GLN	CB-CA-C	-7.86	98.92	111.18
1	C	393	GLN	OE1-CD-NE2	7.79	130.39	122.60
1	A	272	HIS	CB-CG-CD2	-7.75	121.12	131.20
1	D	359	ARG	NE-CZ-NH2	-7.66	112.31	119.20
1	C	146	HIS	CB-CG-CD2	-7.59	121.33	131.20
1	A	270	HIS	N-CA-C	7.58	122.27	112.26
1	D	365	THR	N-CA-C	7.55	120.47	111.33
1	D	205	ARG	NE-CZ-NH2	-7.53	112.43	119.20
1	A	57	GLU	CA-C-N	7.49	129.34	122.37
1	A	57	GLU	C-N-CA	7.49	129.34	122.37
1	D	272	HIS	CB-CG-CD2	-7.43	121.54	131.20
1	B	422	ILE	CB-CA-C	-7.37	104.49	111.05
1	B	205	ARG	NE-CZ-NH2	-7.36	112.58	119.20
1	C	140	ASN	CB-CA-C	-7.32	100.13	109.65
1	C	119	LYS	CA-C-O	7.28	127.19	120.50
1	D	324	ASP	CA-CB-CG	-7.24	105.36	112.60
1	B	205	ARG	NE-CZ-NH1	7.16	128.66	121.50
1	A	404	ASP	CA-CB-CG	-7.16	105.44	112.60
1	A	271	PHE	CA-CB-CG	-7.11	106.69	113.80
1	A	303	SER	CA-C-N	-7.08	112.01	122.35
1	A	303	SER	C-N-CA	-7.08	112.01	122.35
1	B	422	ILE	N-CA-C	7.04	117.18	111.62
1	D	153	PHE	CA-CB-CG	-7.00	106.81	113.80
1	C	157	HIS	CA-CB-CG	-6.99	106.81	113.80
1	A	117	GLN	CB-CA-C	-6.95	99.77	111.02
1	C	160	ASP	N-CA-C	6.94	119.73	111.33
1	B	131	LYS	CA-C-O	6.89	128.27	120.90
1	B	406	PRO	N-CA-CB	6.87	109.43	103.31
1	D	157	HIS	CA-CB-CG	-6.86	106.94	113.80
1	B	270	HIS	N-CA-C	6.85	120.53	112.72
1	D	205	ARG	CD-NE-CZ	6.82	133.95	124.40
1	B	404	ASP	CA-CB-CG	-6.78	105.82	112.60
1	D	33	GLU	CA-C-O	6.76	127.72	120.55
1	C	304	ASP	N-CA-C	6.74	120.84	111.74
1	B	97	PRO	N-CA-C	6.70	122.18	111.26
1	B	328	ARG	NE-CZ-NH1	6.70	128.20	121.50
1	D	380	ARG	CA-C-O	6.68	127.83	120.82
1	D	103	HIS	CA-CB-CG	-6.66	107.14	113.80
1	C	186	THR	CB-CA-C	6.61	118.24	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	200	ASP	N-CA-C	6.58	119.43	109.95
1	A	254	MET	N-CA-C	-6.55	104.22	111.36
1	B	422	ILE	N-CA-CB	-6.47	106.33	111.64
1	B	151	ASP	CA-CB-CG	-6.46	106.14	112.60
1	C	271	PHE	CA-CB-CG	-6.45	107.35	113.80
1	A	28	GLY	CA-C-N	-6.42	115.22	123.19
1	A	28	GLY	C-N-CA	-6.42	115.22	123.19
1	B	176	VAL	CA-C-O	6.41	127.96	121.17
1	A	153	PHE	CA-CB-CG	-6.37	107.43	113.80
1	C	153	PHE	CA-CB-CG	-6.36	107.44	113.80
1	A	359	ARG	NE-CZ-NH2	-6.36	113.48	119.20
1	C	149	SER	CA-C-O	6.29	126.60	119.18
1	D	228	HIS	CB-CA-C	-6.29	98.46	109.02
1	C	207	ALA	CA-C-O	6.28	124.41	118.63
1	D	36	ARG	CA-C-O	6.28	127.42	120.82
1	B	243	GLU	N-CA-C	6.21	118.85	111.71
1	B	206	LEU	N-CA-C	6.19	117.91	111.03
1	A	206	LEU	N-CA-C	6.18	117.89	111.03
1	A	365	THR	N-CA-C	6.17	118.01	111.28
1	B	124	LYS	N-CA-C	6.17	118.01	111.28
1	A	240	ILE	CA-C-N	-6.15	112.16	122.25
1	A	240	ILE	C-N-CA	-6.15	112.16	122.25
1	C	244	SER	N-CA-C	6.15	119.97	112.23
1	B	300	ARG	NE-CZ-NH2	-6.14	113.68	119.20
1	B	103	HIS	CA-CB-CG	-6.12	107.68	113.80
1	D	276	VAL	CA-C-O	6.11	126.84	120.36
1	C	173	SER	CA-C-N	-6.11	111.48	120.28
1	C	173	SER	C-N-CA	-6.11	111.48	120.28
1	D	134	GLN	CB-CA-C	-6.11	103.06	111.73
1	B	48	TRP	N-CA-C	6.10	119.83	112.38
1	D	206	LEU	N-CA-C	6.10	117.80	111.03
1	B	365	THR	N-CA-C	6.09	118.42	111.11
1	A	24	PHE	CA-CB-CG	-6.09	107.71	113.80
1	D	32	GLU	CA-C-N	-6.07	112.14	120.28
1	D	32	GLU	C-N-CA	-6.07	112.14	120.28
1	C	139	PHE	N-CA-C	6.06	118.40	109.24
1	B	34	ALA	CA-C-O	6.05	126.97	120.55
1	C	387	GLN	CB-CA-C	6.05	120.84	110.79
1	D	312	GLU	CA-C-O	6.05	126.93	119.79
1	D	320	ILE	CB-CA-C	-6.05	104.23	111.97
1	C	328	ARG	N-CA-CB	-6.04	100.26	110.41
1	D	331	ILE	CA-C-N	6.03	126.76	121.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	331	ILE	C-N-CA	6.03	126.76	121.58
1	D	243	GLU	N-CA-C	6.01	118.79	111.82
1	C	270	HIS	CA-CB-CG	-6.01	107.79	113.80
1	D	57	GLU	O-C-N	6.00	128.51	122.03
1	A	242	ALA	N-CA-C	-5.96	103.37	110.41
1	A	205	ARG	NE-CZ-NH2	-5.96	113.84	119.20
1	D	324	ASP	N-CA-CB	-5.96	102.97	111.84
1	C	176	VAL	CA-C-O	5.94	127.13	120.95
1	D	313	THR	CA-C-O	5.93	126.70	120.42
1	D	312	GLU	CA-C-N	-5.92	111.88	120.29
1	D	312	GLU	C-N-CA	-5.92	111.88	120.29
1	A	157	HIS	CA-CB-CG	-5.91	107.89	113.80
1	A	140	ASN	CB-CG-ND2	5.91	125.27	116.40
1	B	205	ARG	CD-NE-CZ	5.91	132.67	124.40
1	D	406	PRO	N-CA-CB	5.90	108.58	103.27
1	C	150	ALA	N-CA-C	5.88	118.47	111.71
1	D	188	SER	CA-C-N	-5.88	115.02	122.37
1	D	188	SER	C-N-CA	-5.88	115.02	122.37
1	D	140	ASN	CB-CG-ND2	5.88	125.22	116.40
1	A	57	GLU	O-C-N	5.87	128.37	122.03
1	A	150	ALA	N-CA-C	5.87	118.46	111.71
1	A	229	HIS	N-CA-C	5.87	118.79	108.75
1	B	12	GLN	N-CA-C	-5.87	104.88	111.28
1	A	234	GLU	N-CA-C	5.87	118.29	108.02
1	D	425	ARG	N-CA-C	5.85	120.26	113.18
1	C	228	HIS	N-CA-CB	-5.85	103.12	110.90
1	A	425	ARG	N-CA-C	5.83	120.23	113.18
1	D	328	ARG	NE-CZ-NH2	-5.82	113.96	119.20
1	C	343	ILE	N-CA-C	-5.82	105.06	110.53
1	B	196	ASP	CB-CA-C	-5.80	102.66	109.80
1	B	119	LYS	CA-C-N	5.80	125.93	119.32
1	B	119	LYS	C-N-CA	5.80	125.93	119.32
1	B	370	LYS	O-C-N	-5.80	116.10	122.07
1	D	421	GLU	N-CA-C	5.79	117.68	111.36
1	C	123	PHE	CA-CB-CG	-5.78	108.02	113.80
1	B	116	ASP	CA-CB-CG	-5.78	106.82	112.60
1	C	294	HIS	CB-CA-C	-5.77	101.29	110.81
1	A	390	LEU	N-CA-CB	5.75	116.98	110.03
1	A	135	LEU	CB-CA-C	-5.74	98.02	109.33
1	A	119	LYS	O-C-N	5.72	126.01	121.55
1	A	100	LEU	O-C-N	5.71	130.10	123.30
1	C	327	ASP	N-CA-C	5.71	120.39	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	364	PRO	CB-CA-C	-5.71	105.41	112.89
1	A	134	GLN	CB-CA-C	-5.70	104.22	111.86
1	A	304	ASP	N-CA-C	5.70	119.56	111.92
1	B	117	GLN	N-CA-CB	-5.70	103.28	111.54
1	B	117	GLN	CB-CG-CD	-5.69	102.92	112.60
1	C	89	GLN	CB-CA-C	-5.68	101.95	110.88
1	A	125	ASN	O-C-N	5.68	127.92	122.07
1	D	408	GLY	O-C-N	5.68	129.04	123.31
1	A	304	ASP	CA-CB-CG	-5.67	106.93	112.60
1	D	136	GLY	N-CA-C	-5.66	104.02	113.02
1	A	418	TYR	CA-C-O	5.65	126.41	120.42
1	D	323	HIS	CA-CB-CG	-5.65	108.15	113.80
1	A	17	TRP	CA-C-O	5.63	126.51	120.55
1	B	328	ARG	N-CA-C	5.62	119.98	113.18
1	D	369	ARG	CA-C-O	5.62	126.44	120.10
1	D	340	ILE	CA-CB-CG1	-5.59	100.89	110.40
1	C	49	GLN	CA-C-O	5.59	126.26	119.38
1	D	202	THR	N-CA-CB	-5.59	101.29	110.52
1	C	234	GLU	N-CA-C	5.59	117.52	108.41
1	D	229	HIS	N-CA-C	5.59	118.53	108.48
1	A	272	HIS	CB-CG-ND1	5.58	131.08	122.70
1	D	304	ASP	N-CA-C	5.58	119.39	112.24
1	B	234	GLU	N-CA-C	5.58	117.87	107.99
1	D	254	MET	N-CA-C	-5.58	105.28	111.36
1	C	187	PRO	N-CA-CB	5.57	108.27	103.31
1	B	328	ARG	N-CA-CB	-5.56	101.06	110.41
1	D	234	GLU	N-CA-C	5.54	117.55	108.52
1	D	419	GLU	N-CA-CB	-5.54	101.98	110.01
1	D	334	ASP	N-CA-CB	5.54	121.44	111.36
1	C	57	GLU	O-C-N	5.53	128.00	122.03
1	D	209	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	C	135	LEU	CB-CA-C	-5.52	100.17	109.72
1	A	144	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	180	PHE	CA-CB-CG	5.51	119.31	113.80
1	D	276	VAL	N-CA-C	5.51	116.05	108.12
1	D	386	GLU	CA-C-O	5.51	126.32	120.10
1	B	254	MET	N-CA-C	-5.50	105.20	111.14
1	D	336	PHE	N-CA-CB	5.50	118.40	110.37
1	A	187	PRO	CB-CA-C	-5.50	104.58	111.56
1	B	57	GLU	O-C-N	5.50	128.03	122.09
1	C	357	LEU	CA-C-N	-5.49	112.92	120.28
1	C	357	LEU	C-N-CA	-5.49	112.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	HIS	O-C-N	5.48	129.09	122.35
1	B	89	GLN	CB-CA-C	-5.48	102.28	110.88
1	A	207	ALA	CA-C-O	5.47	123.66	118.63
1	C	182	GLU	N-CA-CB	5.47	117.94	110.01
1	C	369	ARG	CD-NE-CZ	5.47	132.06	124.40
1	D	302	ASP	N-CA-CB	5.47	119.13	110.49
1	B	242	ALA	N-CA-C	-5.45	103.98	110.41
1	C	70	THR	CA-CB-OG1	5.45	117.77	109.60
1	A	87	LEU	CA-C-O	5.44	126.32	120.55
1	B	227	ALA	CA-C-N	-5.44	113.70	122.24
1	B	227	ALA	C-N-CA	-5.44	113.70	122.24
1	B	421	GLU	CA-C-N	-5.44	117.40	123.16
1	B	421	GLU	C-N-CA	-5.44	117.40	123.16
1	A	200	ASP	N-CA-C	5.43	118.13	109.65
1	B	70	THR	CA-CB-OG1	5.43	117.74	109.60
1	B	167	ILE	CB-CA-C	-5.42	104.82	112.14
1	A	320	ILE	N-CA-CB	-5.42	104.21	110.55
1	A	252	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	275	GLU	O-C-N	-5.40	116.64	123.01
1	B	36	ARG	NE-CZ-NH2	-5.40	114.34	119.20
1	C	337	ASP	CB-CG-OD2	-5.37	106.04	118.40
1	A	101	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	396	TRP	CA-C-N	-5.37	112.55	120.28
1	A	396	TRP	C-N-CA	-5.37	112.55	120.28
1	D	240	ILE	CA-C-N	-5.35	112.36	122.05
1	D	240	ILE	C-N-CA	-5.35	112.36	122.05
1	D	244	SER	N-CA-C	5.35	119.52	112.89
1	C	393	GLN	CG-CD-NE2	-5.34	108.38	116.40
1	B	191	ASN	CA-CB-CG	-5.33	107.27	112.60
1	C	323	HIS	CA-CB-CG	-5.33	108.47	113.80
1	D	89	GLN	CA-C-N	-5.32	113.15	120.28
1	D	89	GLN	C-N-CA	-5.32	113.15	120.28
1	A	389	SER	N-CA-CB	5.32	118.62	110.70
1	B	30	ASP	CB-CG-OD2	-5.31	106.18	118.40
1	D	340	ILE	CA-C-N	-5.31	113.16	121.02
1	D	340	ILE	C-N-CA	-5.31	113.16	121.02
1	B	272	HIS	CB-CG-ND1	5.31	130.66	122.70
1	A	276	VAL	N-CA-C	5.30	115.76	108.12
1	D	28	GLY	CA-C-N	-5.30	116.61	123.19
1	D	28	GLY	C-N-CA	-5.30	116.61	123.19
1	B	304	ASP	N-CA-C	5.30	118.89	111.74
1	C	326	PHE	CA-CB-CG	-5.29	108.51	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	THR	N-CA-C	-5.29	105.60	111.36
1	C	195	PRO	CB-CA-C	-5.28	102.20	110.49
1	B	260	ARG	NE-CZ-NH2	-5.28	114.45	119.20
1	D	150	ALA	N-CA-C	5.28	117.72	111.33
1	D	343	ILE	N-CA-C	-5.28	105.39	110.72
1	C	136	GLY	N-CA-C	-5.28	105.54	112.82
1	C	116	ASP	CA-CB-CG	-5.27	107.33	112.60
1	D	37	GLN	N-CA-CB	-5.26	102.38	110.12
1	D	376	ASP	CA-C-N	5.25	128.30	120.31
1	D	376	ASP	C-N-CA	5.25	128.30	120.31
1	A	406	PRO	CA-C-O	-5.25	115.35	121.34
1	A	139	PHE	N-CA-CB	-5.25	103.12	111.62
1	A	322	ARG	CA-C-N	-5.24	114.29	122.73
1	A	322	ARG	C-N-CA	-5.24	114.29	122.73
1	B	150	ALA	N-CA-C	5.24	117.74	111.71
1	C	124	LYS	N-CA-C	5.24	117.67	111.33
1	B	49	GLN	N-CA-C	-5.23	106.16	112.54
1	B	395	VAL	N-CA-C	-5.23	105.61	110.53
1	D	179	TYR	N-CA-CB	-5.23	102.43	110.12
1	A	27	VAL	N-CA-C	-5.23	107.62	112.43
1	C	237	LEU	CA-C-O	5.21	126.13	120.55
1	D	125	ASN	O-C-N	5.21	127.64	122.12
1	C	404	ASP	CA-CB-CG	-5.21	107.39	112.60
1	A	96	GLY	CA-C-N	5.20	125.11	119.76
1	A	96	GLY	C-N-CA	5.20	125.11	119.76
1	B	37	GLN	CB-CG-CD	-5.20	103.76	112.60
1	B	303	SER	N-CA-C	5.19	118.88	112.54
1	B	184	LEU	CA-C-N	-5.19	112.72	121.85
1	B	184	LEU	C-N-CA	-5.19	112.72	121.85
1	B	327	ASP	N-CA-C	5.19	119.67	112.45
1	A	406	PRO	N-CA-CB	5.19	107.93	103.31
1	A	89	GLN	CA-C-O	5.18	126.45	120.90
1	C	183	GLN	N-CA-C	5.18	116.93	111.28
1	D	11	THR	N-CA-CB	5.17	120.30	111.50
1	B	187	PRO	N-CA-CB	5.17	107.91	103.31
1	A	378	THR	CA-CB-CG2	-5.16	101.73	110.50
1	A	100	LEU	N-CA-CB	5.16	119.34	110.68
1	D	173	SER	N-CA-CB	5.16	118.16	110.22
1	A	362	LEU	CA-C-O	5.15	125.38	119.35
1	D	182	GLU	CB-CA-C	-5.15	102.73	110.92
1	A	97	PRO	CB-CA-C	-5.15	104.82	111.46
1	C	117	GLN	CB-CA-C	-5.14	102.41	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	THR	N-CA-CB	5.13	118.95	110.69
1	A	23	ARG	CB-CA-C	-5.13	102.61	110.81
1	D	225	ASN	O-C-N	5.12	125.81	121.20
1	A	337	ASP	CA-C-O	5.12	125.78	120.30
1	A	393	GLN	CB-CA-C	-5.12	101.17	110.63
1	B	57	GLU	CB-CG-CD	-5.12	103.90	112.60
1	D	102	LEU	N-CA-C	5.11	118.08	109.95
1	C	336	PHE	N-CA-CB	5.11	117.83	110.37
1	C	225	ASN	CA-C-N	5.10	124.89	119.28
1	C	225	ASN	C-N-CA	5.10	124.89	119.28
1	D	204	ASP	N-CA-C	5.10	118.50	107.49
1	B	153	PHE	CA-CB-CG	-5.10	108.70	113.80
1	D	217	ASP	CA-CB-CG	-5.10	107.50	112.60
1	C	288	VAL	CB-CA-C	5.09	120.63	111.36
1	A	320	ILE	CA-C-O	5.09	126.57	121.17
1	B	313	THR	CA-C-O	5.09	126.16	120.82
1	C	226	PRO	N-CA-CB	5.09	108.89	103.39
1	D	288	VAL	N-CA-CB	5.09	118.33	111.21
1	B	149	SER	CA-C-O	5.08	125.17	119.18
1	B	140	ASN	CB-CA-C	-5.07	103.06	109.65
1	C	329	VAL	O-C-N	5.07	128.66	123.18
1	D	49	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	C	102	LEU	N-CA-C	5.07	118.33	110.17
1	D	228	HIS	CA-CB-CG	-5.06	108.74	113.80
1	D	252	PHE	CA-CB-CG	-5.06	108.74	113.80
1	B	57	GLU	CB-CA-C	-5.05	102.92	110.90
1	C	272	HIS	CB-CG-ND1	5.05	130.27	122.70
1	A	140	ASN	CB-CG-OD1	-5.04	110.71	120.80
1	A	419	GLU	N-CA-CB	-5.04	102.71	110.12
1	B	50	GLY	N-CA-C	5.04	120.91	114.66
1	B	216	LEU	CA-C-N	-5.04	113.52	120.28
1	B	216	LEU	C-N-CA	-5.04	113.52	120.28
1	D	219	VAL	CA-C-N	-5.02	115.15	122.28
1	D	219	VAL	C-N-CA	-5.02	115.15	122.28
1	D	364	PRO	CB-CA-C	-5.02	106.26	113.09
1	B	173	SER	N-CA-CB	5.02	117.49	110.12
1	A	330	HIS	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3309	0	3231	123	0
1	B	3309	0	3231	135	0
1	C	3309	0	3231	133	0
1	D	3309	0	3231	141	0
2	A	11	0	11	4	0
2	B	11	0	12	0	0
2	C	11	0	12	2	0
2	D	11	0	12	0	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	250	0	0	11	0
5	B	286	0	0	15	0
5	C	263	0	0	9	0
5	D	244	0	0	8	0
All	All	14331	0	12971	507	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 19.

All (507) 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:421:GLU:HG3	1:A:422:ILE:HG12	1.31	1.13
1:B:398:MET:HE2	1:B:402:ARG:HE	1.11	1.12
1:D:398:MET:HE2	1:D:402:ARG:HE	1.13	1.12
1:C:398:MET:HE2	1:C:402:ARG:HE	1.08	1.12
1:A:398:MET:HE2	1:A:402:ARG:HE	1.11	1.06
1:A:393:GLN:NE2	1:D:393:GLN:HE22	1.53	1.05
1:A:393:GLN:HE22	1:D:393:GLN:NE2	1.57	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:SER:H	1:D:169:HIS:HE1	1.12	0.98
1:C:114:SER:HB3	1:C:117:GLN:HG3	1.47	0.96
1:D:421:GLU:HG3	1:D:422:ILE:HG12	1.47	0.95
1:B:79:ASN:ND2	1:B:82:GLU:H	1.65	0.94
1:B:393:GLN:HE22	1:C:393:GLN:NE2	1.65	0.94
1:A:119:LYS:H	1:A:122:HIS:HD2	1.14	0.94
1:B:45:MET:HE3	1:B:98:LYS:HB3	1.49	0.94
1:D:398:MET:HE2	1:D:402:ARG:NE	1.82	0.93
1:B:393:GLN:HE22	1:C:393:GLN:HE22	1.08	0.93
1:A:393:GLN:HE22	1:D:393:GLN:HE22	1.00	0.92
1:C:79:ASN:ND2	1:C:82:GLU:H	1.67	0.92
1:B:393:GLN:NE2	1:C:393:GLN:HE22	1.69	0.91
1:A:369:ARG:HH11	1:A:369:ARG:HG3	1.32	0.91
1:C:119:LYS:H	1:C:122:HIS:CD2	1.89	0.91
1:A:119:LYS:H	1:A:122:HIS:CD2	1.88	0.91
1:A:398:MET:HE2	1:A:402:ARG:NE	1.87	0.90
1:C:119:LYS:H	1:C:122:HIS:HD2	1.08	0.90
1:D:119:LYS:H	1:D:122:HIS:CD2	1.91	0.89
1:B:119:LYS:H	1:B:122:HIS:HD2	1.17	0.89
1:A:55:GLY:HA3	1:A:105:ILE:HD12	1.53	0.89
1:B:421:GLU:HG3	1:B:422:ILE:HG12	1.55	0.89
1:D:369:ARG:HG3	1:D:369:ARG:HH11	1.37	0.89
1:A:45:MET:HE3	1:A:98:LYS:HB3	1.55	0.88
1:A:45:MET:HE1	1:A:98:LYS:HD2	1.56	0.87
1:B:45:MET:HE3	1:B:98:LYS:CB	2.05	0.85
1:B:114:SER:HB3	1:B:117:GLN:HG3	1.59	0.85
1:B:295:VAL:HG12	1:B:307:VAL:HG21	1.57	0.85
1:C:45:MET:HE3	1:C:98:LYS:CB	2.07	0.85
1:D:45:MET:HE3	1:D:98:LYS:HB3	1.59	0.84
1:B:369:ARG:HG3	1:B:369:ARG:HH11	1.43	0.84
1:A:142:SER:H	1:A:169:HIS:HE1	1.23	0.84
1:B:119:LYS:H	1:B:122:HIS:CD2	1.95	0.84
1:A:79:ASN:ND2	1:A:82:GLU:H	1.74	0.84
1:C:45:MET:HE3	1:C:98:LYS:HB3	1.60	0.83
1:C:398:MET:HE2	1:C:402:ARG:NE	1.90	0.83
1:A:45:MET:CE	1:A:98:LYS:HD2	2.08	0.83
1:D:314:GLN:HE21	1:D:359:ARG:HH11	1.24	0.82
1:B:45:MET:HE1	1:B:98:LYS:HD2	1.59	0.82
1:A:45:MET:HE3	1:A:98:LYS:CB	2.10	0.82
1:D:76:LYS:HE3	5:D:4537:HOH:O	1.81	0.81
1:D:119:LYS:H	1:D:122:HIS:HD2	1.25	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:MET:HE3	1:D:98:LYS:CB	2.10	0.81
1:B:45:MET:CE	1:B:98:LYS:HD2	2.09	0.81
1:C:76:LYS:HE3	5:C:3486:HOH:O	1.79	0.80
1:C:142:SER:H	1:C:169:HIS:HE1	1.28	0.80
1:A:114:SER:HB3	1:A:117:GLN:HG3	1.62	0.80
1:C:205:ARG:HD2	5:C:3580:HOH:O	1.80	0.80
1:A:124:LYS:O	1:A:128:GLU:HG3	1.81	0.80
1:D:134:GLN:HA	1:D:134:GLN:HE21	1.45	0.80
1:B:205:ARG:HD2	5:B:2606:HOH:O	1.79	0.80
1:B:134:GLN:HA	1:B:134:GLN:HE21	1.47	0.80
1:B:33:GLU:HG2	5:B:2491:HOH:O	1.82	0.79
1:A:314:GLN:HE21	1:A:359:ARG:HH11	1.31	0.79
1:D:142:SER:N	1:D:169:HIS:HE1	1.80	0.79
1:A:367:GLU:HG3	5:A:1491:HOH:O	1.83	0.79
1:A:393:GLN:HB2	5:A:1692:HOH:O	1.82	0.79
1:D:367:GLU:HG3	5:D:4501:HOH:O	1.81	0.79
1:D:398:MET:CE	1:D:402:ARG:HG3	2.13	0.79
1:B:295:VAL:HG12	1:B:307:VAL:CG2	2.14	0.78
1:D:18:GLU:O	1:D:22:GLN:HG3	1.83	0.78
1:B:336:PHE:HB2	5:B:2744:HOH:O	1.82	0.78
1:B:398:MET:HE2	1:B:402:ARG:NE	1.96	0.78
1:C:134:GLN:HE21	1:C:134:GLN:HA	1.47	0.77
1:D:142:SER:H	1:D:169:HIS:CE1	2.01	0.77
1:D:205:ARG:HD2	5:D:4553:HOH:O	1.84	0.77
1:B:142:SER:H	1:B:169:HIS:HE1	1.30	0.77
1:B:269:GLY:HA2	1:B:298:PRO:HG3	1.66	0.77
1:D:45:MET:CE	1:D:98:LYS:HD2	2.14	0.77
1:D:373:ALA:HB3	1:D:374:PRO:HD2	1.69	0.75
1:C:45:MET:CE	1:C:98:LYS:HD2	2.16	0.75
1:B:398:MET:HE3	1:B:402:ARG:HG3	1.68	0.75
1:D:49:GLN:HE22	1:D:337:ASP:H	1.32	0.74
1:C:49:GLN:HE22	1:C:337:ASP:H	1.35	0.73
1:D:79:ASN:ND2	1:D:82:GLU:H	1.86	0.73
1:A:142:SER:N	1:A:169:HIS:HE1	1.87	0.73
1:B:398:MET:CE	1:B:402:ARG:HE	1.97	0.72
1:A:76:LYS:HE3	5:A:1503:HOH:O	1.89	0.72
1:D:295:VAL:HG12	1:D:307:VAL:HG21	1.71	0.72
1:D:89:GLN:NE2	5:D:4524:HOH:O	2.23	0.71
1:A:121:GLU:HA	1:A:124:LYS:HE3	1.72	0.71
1:B:142:SER:N	1:B:169:HIS:HE1	1.89	0.70
1:A:205:ARG:HD2	5:A:1537:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLU:HA	1:B:124:LYS:HE3	1.74	0.69
1:C:114:SER:HB3	1:C:117:GLN:CG	2.20	0.69
1:C:295:VAL:HG12	1:C:307:VAL:HG21	1.73	0.69
1:A:369:ARG:HG3	1:A:369:ARG:NH1	2.04	0.69
1:B:289:PRO:O	1:B:328:ARG:HD2	1.92	0.69
1:D:11:THR:N	5:D:4498:HOH:O	2.26	0.69
1:D:365:THR:O	1:D:369:ARG:HB2	1.92	0.68
1:D:314:GLN:NE2	1:D:359:ARG:HD3	2.09	0.67
1:C:398:MET:HE3	1:C:402:ARG:HG3	1.75	0.67
1:C:295:VAL:HG12	1:C:307:VAL:CG2	2.24	0.67
1:A:373:ALA:HB3	1:A:374:PRO:HD2	1.75	0.67
1:B:139:PHE:HE2	1:B:173:SER:HB3	1.59	0.67
1:C:314:GLN:HE21	1:C:359:ARG:HH11	1.43	0.67
1:C:398:MET:CE	1:C:402:ARG:HE	1.97	0.67
1:C:421:GLU:HG3	1:C:422:ILE:HG12	1.75	0.67
1:D:369:ARG:HG3	1:D:369:ARG:NH1	2.05	0.67
1:C:121:GLU:HA	1:C:124:LYS:CE	2.25	0.66
1:B:139:PHE:CE2	1:B:173:SER:HB3	2.31	0.66
1:B:398:MET:HE3	1:B:402:ARG:CG	2.26	0.66
1:D:134:GLN:HE21	1:D:134:GLN:CA	2.08	0.66
1:D:289:PRO:O	1:D:328:ARG:HD2	1.96	0.66
1:D:398:MET:HE3	1:D:402:ARG:HG3	1.76	0.66
1:A:89:GLN:NE2	5:A:1481:HOH:O	2.29	0.66
1:B:121:GLU:HA	1:B:124:LYS:CE	2.25	0.65
1:A:79:ASN:HD21	1:A:82:GLU:H	1.43	0.65
1:D:45:MET:HE1	1:D:98:LYS:HD2	1.76	0.65
1:D:121:GLU:HA	1:D:124:LYS:HE3	1.78	0.65
1:B:373:ALA:HB3	1:B:374:PRO:HD2	1.77	0.65
1:C:373:ALA:HB3	1:C:374:PRO:HD2	1.79	0.65
1:D:314:GLN:HE22	1:D:359:ARG:HD3	1.60	0.65
1:B:49:GLN:HE22	1:B:337:ASP:H	1.44	0.65
1:C:369:ARG:HH11	1:D:204:ASP:HB2	1.62	0.65
1:A:142:SER:H	1:A:169:HIS:CE1	2.10	0.64
1:A:365:THR:O	1:A:369:ARG:HB2	1.96	0.64
1:A:314:GLN:NE2	1:A:359:ARG:HH11	1.95	0.64
1:B:18:GLU:O	1:B:22:GLN:HG3	1.98	0.64
1:C:55:GLY:HA3	1:C:105:ILE:HD12	1.80	0.64
1:C:146:HIS:CG	1:C:147:PRO:HD2	2.33	0.64
1:C:421:GLU:HB2	5:C:3721:HOH:O	1.96	0.64
1:B:45:MET:HE2	1:B:350:THR:HG21	1.79	0.64
1:C:18:GLU:O	1:C:22:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLN:HE22	1:D:393:GLN:CD	2.06	0.63
1:B:393:GLN:HG2	1:C:389:SER:C	2.23	0.63
1:D:119:LYS:HB3	1:D:120:PRO:HD2	1.80	0.63
1:A:124:LYS:HD3	1:A:179:TYR:OH	1.98	0.63
1:B:124:LYS:O	1:B:128:GLU:HG3	1.97	0.63
1:C:142:SER:N	1:C:169:HIS:HE1	1.97	0.63
1:C:119:LYS:N	1:C:122:HIS:HD2	1.90	0.62
1:D:295:VAL:HG12	1:D:307:VAL:CG2	2.29	0.62
1:C:387:GLN:OE1	5:C:3593:HOH:O	2.16	0.62
1:C:406:PRO:HG2	1:C:411:TRP:HB3	1.82	0.62
1:C:387:GLN:HG2	5:C:3570:HOH:O	1.99	0.62
1:A:289:PRO:O	1:A:328:ARG:HD2	2.00	0.62
1:B:389:SER:C	1:C:393:GLN:HG2	2.25	0.62
1:C:170:CYS:O	1:C:174:ARG:HG3	2.00	0.61
1:B:370:LYS:O	1:B:374:PRO:HD2	2.00	0.61
1:D:124:LYS:O	1:D:128:GLU:HG3	2.01	0.61
1:A:121:GLU:HA	1:A:124:LYS:CE	2.29	0.61
1:A:134:GLN:HA	1:A:134:GLN:HE21	1.65	0.61
1:B:421:GLU:HB2	5:B:2722:HOH:O	1.99	0.61
1:D:55:GLY:HA3	1:D:105:ILE:HD12	1.82	0.61
1:D:79:ASN:HD22	1:D:81:SER:N	1.98	0.61
1:B:79:ASN:HD21	1:B:82:GLU:H	1.47	0.61
1:A:295:VAL:HG12	1:A:307:VAL:HG21	1.83	0.60
1:B:369:ARG:HG3	1:B:369:ARG:NH1	2.11	0.60
1:C:314:GLN:HE22	1:C:359:ARG:HD3	1.66	0.60
1:A:71:GLY:HA3	1:A:339:SER:HA	1.83	0.60
1:B:367:GLU:HG3	5:B:2509:HOH:O	2.02	0.60
1:B:369:ARG:NE	5:B:2500:HOH:O	2.34	0.60
1:C:370:LYS:O	1:C:374:PRO:HD2	2.02	0.60
1:A:207:ALA:HB3	1:A:208:PRO:HD3	1.83	0.60
1:C:314:GLN:NE2	1:C:359:ARG:HD3	2.17	0.60
1:D:79:ASN:HD21	1:D:82:GLU:H	1.49	0.60
1:D:314:GLN:HE21	1:D:359:ARG:NH1	1.99	0.60
1:C:120:PRO:HB3	1:C:179:TYR:CD2	2.37	0.60
1:A:314:GLN:HE21	1:A:359:ARG:NH1	1.98	0.60
1:A:406:PRO:HG2	1:A:411:TRP:HB3	1.85	0.59
1:D:398:MET:HE2	1:D:402:ARG:HG3	1.82	0.59
1:C:119:LYS:N	1:C:122:HIS:CD2	2.67	0.59
1:C:124:LYS:O	1:C:128:GLU:HG3	2.01	0.59
1:A:314:GLN:HE22	1:A:359:ARG:HD3	1.66	0.59
1:C:45:MET:CE	1:C:98:LYS:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ASN:HD21	1:C:82:GLU:H	1.46	0.59
1:C:121:GLU:HA	1:C:124:LYS:HE3	1.83	0.59
1:A:393:GLN:CD	1:D:393:GLN:HE22	2.08	0.59
1:A:55:GLY:CA	1:A:105:ILE:HD12	2.31	0.59
1:D:416:ARG:O	1:D:419:GLU:HB3	2.03	0.59
1:A:128:GLU:HG2	5:A:1473:HOH:O	2.04	0.58
1:B:55:GLY:HA3	1:B:105:ILE:HD12	1.84	0.58
1:D:139:PHE:CE2	1:D:173:SER:HB3	2.39	0.58
1:D:387:GLN:HG2	5:D:4582:HOH:O	2.04	0.58
1:A:123:PHE:HA	5:A:1622:HOH:O	2.04	0.58
1:A:236:LYS:NZ	2:A:1462:RNS:O1	2.28	0.58
1:C:120:PRO:HB3	1:C:179:TYR:CG	2.38	0.58
1:B:142:SER:H	1:B:169:HIS:CE1	2.17	0.58
1:B:114:SER:HB3	1:B:117:GLN:CG	2.34	0.58
1:D:37:GLN:OE1	1:D:40:ARG:HD3	2.03	0.58
1:A:295:VAL:HG12	1:A:307:VAL:CG2	2.33	0.58
1:C:368:LEU:HD21	1:C:383:LEU:HB3	1.85	0.57
1:C:398:MET:HE3	1:C:402:ARG:CG	2.35	0.57
1:B:167:ILE:HG22	1:B:171:LYS:HD2	1.87	0.57
1:D:285:MET:CE	1:D:325:LEU:HD21	2.34	0.57
1:A:79:ASN:C	1:A:79:ASN:HD22	2.13	0.57
1:D:121:GLU:HA	1:D:124:LYS:CE	2.34	0.57
1:D:406:PRO:HG2	1:D:411:TRP:HB3	1.86	0.57
1:D:225:ASN:HB3	1:D:228:HIS:ND1	2.20	0.57
1:B:146:HIS:CG	1:B:147:PRO:HD2	2.40	0.56
1:D:114:SER:HB3	1:D:117:GLN:HG3	1.88	0.56
1:A:314:GLN:NE2	1:A:359:ARG:HD3	2.21	0.56
1:B:151:ASP:HB2	5:B:2652:HOH:O	2.05	0.56
1:D:139:PHE:HE2	1:D:173:SER:HB3	1.70	0.55
1:C:116:ASP:OD1	1:C:117:GLN:HG2	2.07	0.55
1:D:45:MET:CE	1:D:98:LYS:HB3	2.35	0.55
1:D:79:ASN:ND2	1:D:81:SER:HB2	2.22	0.55
1:D:119:LYS:O	1:D:122:HIS:N	2.36	0.55
1:D:314:GLN:NE2	1:D:359:ARG:HH11	1.99	0.55
1:B:225:ASN:HB3	1:B:228:HIS:ND1	2.22	0.55
1:A:24:PHE:O	1:A:27:VAL:HG22	2.07	0.54
1:A:71:GLY:HA3	1:A:339:SER:CA	2.36	0.54
1:B:79:ASN:HD22	1:B:81:SER:N	2.05	0.54
1:C:152:GLY:O	1:C:196:ASP:HA	2.06	0.54
1:D:157:HIS:O	1:D:163:ARG:HD3	2.07	0.54
1:A:49:GLN:HE22	1:A:337:ASP:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:HD22	1:B:82:GLU:H	1.50	0.54
1:B:406:PRO:HG2	1:B:411:TRP:HB3	1.89	0.54
1:A:299:VAL:HG12	1:C:243:GLU:HB3	1.89	0.54
1:C:290:GLN:HG2	1:C:330:HIS:NE2	2.22	0.54
1:B:207:ALA:HB3	1:B:208:PRO:HD3	1.90	0.54
1:C:289:PRO:O	1:C:328:ARG:HD2	2.08	0.54
1:D:146:HIS:CG	1:D:147:PRO:HD2	2.43	0.54
1:A:114:SER:HB3	1:A:117:GLN:CG	2.35	0.53
1:C:181:GLY:HA2	1:C:186:THR:O	2.08	0.53
1:A:79:ASN:ND2	1:A:82:GLU:HG3	2.23	0.53
1:A:141:PRO:HD2	1:A:191:ASN:O	2.07	0.53
1:B:314:GLN:HE21	1:B:359:ARG:HH11	1.56	0.53
1:A:121:GLU:CA	1:A:124:LYS:HE3	2.38	0.53
1:A:370:LYS:O	1:A:374:PRO:HD2	2.09	0.53
1:A:410:GLU:CD	1:A:410:GLU:H	2.15	0.53
1:C:383:LEU:HD23	1:C:383:LEU:N	2.23	0.53
1:A:120:PRO:HB3	1:A:179:TYR:CG	2.43	0.53
1:D:181:GLY:HA2	1:D:186:THR:O	2.08	0.53
1:A:119:LYS:N	1:A:122:HIS:CD2	2.69	0.53
1:A:393:GLN:HG2	1:D:389:SER:C	2.34	0.53
1:B:79:ASN:ND2	1:B:82:GLU:N	2.47	0.53
1:C:369:ARG:NH1	1:D:204:ASP:HB2	2.23	0.53
1:B:45:MET:CE	1:B:98:LYS:HB3	2.31	0.52
1:B:120:PRO:HB3	1:B:179:TYR:CD2	2.44	0.52
1:C:37:GLN:OE1	1:C:40:ARG:HD3	2.10	0.52
1:A:270:HIS:NE2	2:A:1462:RNS:O2	2.41	0.52
1:B:57:GLU:HB2	5:B:2633:HOH:O	2.08	0.52
1:C:225:ASN:OD1	1:C:226:PRO:HD2	2.10	0.52
1:A:18:GLU:O	1:A:22:GLN:HG3	2.10	0.52
1:D:37:GLN:O	1:D:40:ARG:HB2	2.10	0.51
1:D:373:ALA:CB	1:D:374:PRO:HD2	2.32	0.51
1:B:120:PRO:HB3	1:B:179:TYR:CG	2.45	0.51
1:B:89:GLN:NE2	5:B:2507:HOH:O	2.43	0.51
1:D:370:LYS:O	1:D:374:PRO:HD2	2.10	0.51
1:C:267:ASP:HA	1:C:294:HIS:HB2	1.92	0.51
1:C:390:LEU:HB3	1:C:391:PRO:HD2	1.92	0.51
1:A:121:GLU:HA	1:A:124:LYS:CG	2.41	0.51
1:A:45:MET:HE2	1:A:350:THR:HG21	1.92	0.51
1:B:152:GLY:O	1:B:196:ASP:HA	2.10	0.51
1:C:79:ASN:HD22	1:C:81:SER:N	2.09	0.51
1:D:89:GLN:HG2	1:D:418:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HD2	1:A:129:TRP:CD1	2.46	0.51
1:C:369:ARG:HH11	1:C:369:ARG:HG3	1.75	0.51
1:B:267:ASP:HA	1:B:294:HIS:HB2	1.94	0.50
1:B:119:LYS:N	1:B:122:HIS:CD2	2.75	0.50
1:C:236:LYS:HE2	1:C:238:PHE:O	2.12	0.50
1:A:57:GLU:HB2	5:A:1623:HOH:O	2.11	0.50
1:C:142:SER:H	1:C:169:HIS:CE1	2.18	0.50
1:D:84:ARG:HD2	1:D:129:TRP:CD1	2.47	0.50
1:D:234:GLU:OE2	1:D:267:ASP:HB2	2.12	0.50
1:B:213:LEU:HD11	1:B:260:ARG:NH2	2.27	0.49
1:B:301:TRP:O	1:B:303:SER:N	2.37	0.49
1:C:121:GLU:HA	1:C:124:LYS:CG	2.42	0.49
1:A:299:VAL:CG1	1:C:243:GLU:HB3	2.43	0.49
1:C:234:GLU:OE2	1:C:267:ASP:HB2	2.12	0.49
1:A:233:VAL:HB	1:A:253:TYR:CD1	2.47	0.49
1:C:370:LYS:O	1:C:374:PRO:HG2	2.12	0.49
1:C:134:GLN:HE21	1:C:134:GLN:CA	2.18	0.49
1:D:115:ARG:O	1:D:169:HIS:HD2	1.95	0.49
1:D:141:PRO:HD2	1:D:191:ASN:O	2.12	0.49
1:D:387:GLN:OE1	5:D:4638:HOH:O	2.19	0.49
1:A:270:HIS:HE1	2:A:1462:RNS:H2	1.77	0.49
1:B:335:PHE:C	1:B:336:PHE:CD2	2.91	0.49
1:A:387:GLN:HG2	5:A:1587:HOH:O	2.13	0.49
1:D:151:ASP:HB2	5:D:4606:HOH:O	2.12	0.49
5:A:1650:HOH:O	1:D:377:TYR:HB2	2.12	0.49
1:D:207:ALA:HB3	1:D:208:PRO:HD3	1.94	0.49
1:A:115:ARG:O	1:A:169:HIS:HD2	1.95	0.48
1:A:419:GLU:O	1:A:424:SER:HB3	2.13	0.48
1:B:79:ASN:HD22	1:B:79:ASN:C	2.20	0.48
1:C:119:LYS:O	1:C:122:HIS:N	2.27	0.48
1:D:373:ALA:CB	1:D:374:PRO:CD	2.91	0.48
1:B:370:LYS:O	1:B:374:PRO:HG2	2.13	0.48
1:C:204:ASP:HB2	1:D:369:ARG:NH1	2.29	0.48
1:C:335:PHE:C	1:C:336:PHE:CD2	2.91	0.48
1:C:45:MET:HE1	1:C:98:LYS:HD2	1.94	0.48
1:D:84:ARG:O	1:D:88:GLU:HG3	2.14	0.48
1:B:318:SER:O	1:B:322:ARG:HG3	2.14	0.48
1:C:124:LYS:HD3	1:C:179:TYR:OH	2.14	0.48
1:D:398:MET:HE2	1:D:402:ARG:CG	2.42	0.48
1:C:213:LEU:HD11	1:C:260:ARG:NH2	2.29	0.48
1:B:243:GLU:HB3	1:D:299:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLN:NE2	1:D:393:GLN:NE2	2.29	0.47
1:B:57:GLU:HG2	5:B:2668:HOH:O	2.14	0.47
1:C:96:GLY:HA2	1:C:403:HIS:CE1	2.48	0.47
1:B:96:GLY:HA2	1:B:403:HIS:CE1	2.49	0.47
1:B:79:ASN:ND2	1:B:81:SER:HB2	2.29	0.47
1:A:17:TRP:CH2	1:A:31:VAL:HG23	2.49	0.47
1:B:121:GLU:HA	1:B:124:LYS:CG	2.45	0.47
1:B:121:GLU:HB3	5:B:2645:HOH:O	2.13	0.47
1:B:234:GLU:OE2	1:B:267:ASP:HB2	2.14	0.47
1:B:368:LEU:HD21	1:B:383:LEU:HB3	1.95	0.47
1:B:393:GLN:CD	1:C:393:GLN:HE22	2.20	0.47
1:D:46:HIS:ND1	1:D:333:LEU:HB2	2.29	0.47
1:D:370:LYS:O	1:D:374:PRO:HG2	2.14	0.47
1:B:213:LEU:C	1:B:213:LEU:HD12	2.40	0.47
1:C:213:LEU:C	1:C:213:LEU:HD12	2.39	0.47
1:A:213:LEU:HD11	1:A:260:ARG:NH2	2.30	0.47
1:D:194:ILE:HD12	1:D:196:ASP:CG	2.39	0.47
1:B:384:LEU:O	1:B:387:GLN:HB3	2.15	0.47
1:C:46:HIS:NE2	1:C:49:GLN:HB2	2.29	0.47
1:C:115:ARG:O	1:C:169:HIS:HD2	1.98	0.47
1:A:304:ASP:HB3	1:A:336:PHE:H	1.79	0.47
1:C:79:ASN:HD22	1:C:82:GLU:H	1.54	0.47
1:C:383:LEU:HA	1:C:383:LEU:HD22	1.17	0.47
1:D:383:LEU:N	1:D:383:LEU:HD23	2.29	0.47
1:D:108:GLU:OE2	1:D:125:ASN:HB2	2.15	0.47
1:D:152:GLY:O	1:D:196:ASP:HA	2.15	0.47
1:A:134:GLN:HE21	1:A:134:GLN:CA	2.28	0.46
1:A:89:GLN:HG3	1:A:418:TYR:CG	2.50	0.46
1:A:146:HIS:CG	1:A:147:PRO:HD2	2.49	0.46
1:D:17:TRP:CH2	1:D:31:VAL:HG23	2.50	0.46
1:D:79:ASN:ND2	1:D:82:GLU:HG3	2.30	0.46
1:D:265:CYS:HA	1:D:292:LEU:O	2.15	0.46
1:A:373:ALA:CB	1:A:374:PRO:HD2	2.39	0.46
1:A:418:TYR:O	1:A:422:ILE:HB	2.15	0.46
1:B:157:HIS:O	1:B:163:ARG:HD3	2.16	0.46
1:D:84:ARG:HD2	1:D:129:TRP:CG	2.50	0.46
1:D:176:VAL:O	1:D:179:TYR:HB3	2.16	0.46
1:A:119:LYS:N	1:A:122:HIS:HD2	1.97	0.46
1:C:45:MET:HE1	1:C:91:MET:HG2	1.98	0.46
1:A:351:ARG:O	1:A:355:LYS:HG3	2.16	0.46
1:D:290:GLN:HG2	1:D:330:HIS:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:HG3	1:A:418:TYR:CD1	2.50	0.46
1:B:393:GLN:HE22	1:C:393:GLN:CD	2.22	0.46
1:D:79:ASN:HD22	1:D:79:ASN:C	2.24	0.46
1:C:70:THR:N	5:C:3529:HOH:O	2.28	0.46
1:C:46:HIS:ND1	1:C:333:LEU:HB2	2.31	0.45
1:B:365:THR:O	1:B:369:ARG:HB2	2.16	0.45
1:D:383:LEU:HD22	1:D:383:LEU:HA	1.51	0.45
1:C:119:LYS:O	1:C:120:PRO:C	2.59	0.45
1:D:335:PHE:C	1:D:336:PHE:CD2	2.94	0.45
1:A:51:ASP:OD2	1:A:55:GLY:N	2.44	0.45
1:A:213:LEU:CD1	1:A:256:TYR:HE1	2.30	0.45
1:B:134:GLN:HE21	1:B:134:GLN:CA	2.20	0.45
1:B:389:SER:O	1:C:393:GLN:HG2	2.16	0.45
1:C:13:LEU:HD21	1:C:398:MET:HA	1.99	0.45
1:A:398:MET:O	1:A:402:ARG:HG3	2.16	0.45
1:B:49:GLN:NE2	1:B:336:PHE:HA	2.31	0.45
1:B:213:LEU:HD12	1:B:213:LEU:O	2.16	0.45
1:A:46:HIS:ND1	1:A:46:HIS:N	2.58	0.45
1:B:116:ASP:OD1	1:B:117:GLN:HG2	2.17	0.45
1:C:207:ALA:HB3	1:C:208:PRO:HD3	1.98	0.45
1:D:79:ASN:HD22	1:D:81:SER:H	1.65	0.45
1:D:11:THR:HG23	1:D:12:GLN:N	2.31	0.45
1:A:373:ALA:CB	1:A:374:PRO:CD	2.96	0.45
1:B:78:ARG:N	1:B:82:GLU:OE1	2.46	0.45
1:B:115:ARG:HB3	1:B:169:HIS:CD2	2.52	0.45
1:A:181:GLY:HA2	1:A:186:THR:O	2.17	0.44
1:B:37:GLN:OE1	1:B:40:ARG:HD3	2.18	0.44
1:C:27:VAL:O	1:C:27:VAL:HG23	2.17	0.44
1:B:181:GLY:HA3	1:B:228:HIS:O	2.17	0.44
1:C:119:LYS:HB3	1:C:120:PRO:HD2	1.99	0.44
1:B:181:GLY:HA2	1:B:186:THR:O	2.18	0.44
1:C:79:ASN:HD22	1:C:79:ASN:C	2.26	0.44
1:C:216:LEU:O	1:C:220:ILE:HG12	2.18	0.44
1:D:120:PRO:HB3	1:D:179:TYR:CG	2.53	0.44
1:A:251:GLU:H	1:A:251:GLU:CD	2.25	0.44
1:D:75:GLY:O	1:D:76:LYS:C	2.60	0.44
1:B:211:ARG:NH1	5:B:2642:HOH:O	2.48	0.44
1:C:78:ARG:HB2	1:C:82:GLU:OE1	2.18	0.44
1:C:204:ASP:HB2	1:D:369:ARG:HH11	1.83	0.44
1:D:383:LEU:O	1:D:384:LEU:C	2.60	0.44
1:D:37:GLN:OE1	1:D:37:GLN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LYS:CB	1:D:120:PRO:HD2	2.44	0.44
1:D:225:ASN:OD1	1:D:226:PRO:HD2	2.17	0.44
1:B:373:ALA:CB	1:B:374:PRO:CD	2.95	0.43
1:C:295:VAL:HG21	1:C:353:MET:SD	2.58	0.43
1:D:24:PHE:O	1:D:27:VAL:HG22	2.18	0.43
1:D:27:VAL:O	1:D:27:VAL:HG23	2.16	0.43
1:D:86:ASP:HB3	1:D:343:ILE:HD11	1.99	0.43
1:D:269:GLY:HA2	1:D:298:PRO:HG3	1.99	0.43
1:A:200:ASP:O	1:A:201:ILE:C	2.59	0.43
1:A:213:LEU:CD1	1:A:256:TYR:CE1	3.01	0.43
1:A:241:GLY:H	1:A:243:GLU:CD	2.25	0.43
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.84	0.43
1:D:71:GLY:HA3	1:D:339:SER:CA	2.48	0.43
1:D:390:LEU:HB3	1:D:391:PRO:HD2	2.00	0.43
1:D:408:GLY:O	1:D:411:TRP:HD1	2.01	0.43
1:A:120:PRO:HB3	1:A:179:TYR:CD2	2.53	0.43
1:C:79:ASN:ND2	1:C:82:GLU:N	2.50	0.43
1:C:269:GLY:HA2	1:C:298:PRO:HG3	1.99	0.43
1:D:79:ASN:ND2	1:D:79:ASN:C	2.77	0.43
1:B:205:ARG:HG2	1:B:245:TYR:CD1	2.53	0.43
1:C:297:ARG:O	1:C:305:HIS:HB2	2.18	0.43
1:D:405:THR:HG23	1:D:406:PRO:HD2	2.00	0.43
1:C:387:GLN:HB2	5:C:3593:HOH:O	2.18	0.43
1:A:389:SER:C	1:D:393:GLN:HG2	2.44	0.43
1:B:79:ASN:HD21	1:B:82:GLU:N	2.13	0.43
1:B:236:LYS:HE2	1:B:238:PHE:O	2.19	0.43
1:C:139:PHE:HE2	1:C:173:SER:HB3	1.84	0.43
1:B:115:ARG:O	1:B:169:HIS:HD2	2.02	0.43
1:B:301:TRP:C	1:B:303:SER:N	2.75	0.43
1:C:71:GLY:HA3	1:C:339:SER:CA	2.48	0.43
1:D:11:THR:CG2	1:D:12:GLN:N	2.81	0.43
1:A:79:ASN:ND2	1:A:79:ASN:C	2.77	0.43
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.84	0.43
1:C:373:ALA:CB	1:C:374:PRO:HD2	2.44	0.43
1:D:79:ASN:HD21	1:D:81:SER:HB2	1.84	0.42
1:D:134:GLN:CA	1:D:134:GLN:NE2	2.79	0.42
1:A:213:LEU:HD12	1:A:213:LEU:O	2.19	0.42
1:A:225:ASN:HB3	1:A:228:HIS:ND1	2.33	0.42
1:C:71:GLY:HA3	1:C:339:SER:HA	2.00	0.42
1:D:335:PHE:C	1:D:335:PHE:CD1	2.97	0.42
1:A:76:LYS:HG3	1:A:77:ALA:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ALA:HB2	1:B:86:ASP:OD2	2.18	0.42
1:B:290:GLN:HG2	1:B:330:HIS:NE2	2.35	0.42
1:D:355:LYS:HE3	1:D:396:TRP:NE1	2.34	0.42
1:A:79:ASN:HD21	1:A:82:GLU:HG3	1.84	0.42
1:A:116:ASP:HA	1:A:169:HIS:HA	2.00	0.42
1:A:335:PHE:C	1:A:336:PHE:CD2	2.97	0.42
1:B:36:ARG:NH2	5:B:2603:HOH:O	2.27	0.42
1:C:84:ARG:HD2	1:C:129:TRP:CD1	2.54	0.42
1:C:373:ALA:HB3	1:C:374:PRO:CD	2.49	0.42
1:D:71:GLY:HA3	1:D:339:SER:HA	2.00	0.42
1:D:119:LYS:N	1:D:122:HIS:CD2	2.73	0.42
1:D:241:GLY:H	1:D:243:GLU:CD	2.26	0.42
1:A:270:HIS:CE1	2:A:1462:RNS:H2	2.55	0.42
1:B:290:GLN:HG3	1:B:328:ARG:HA	2.02	0.42
1:C:410:GLU:O	1:C:411:TRP:C	2.60	0.42
1:A:130:ALA:O	1:A:131:LYS:C	2.61	0.42
1:B:325:LEU:HA	1:B:325:LEU:HD23	1.62	0.42
1:C:213:LEU:HD12	1:C:213:LEU:O	2.20	0.42
1:C:373:ALA:CB	1:C:374:PRO:CD	2.97	0.42
1:A:89:GLN:CG	1:A:418:TYR:CD1	3.03	0.42
1:C:193:TRP:CD2	2:C:3462:RNS:H3	2.55	0.42
1:D:78:ARG:N	1:D:82:GLU:OE1	2.52	0.42
1:B:374:PRO:CD	5:B:2631:HOH:O	2.67	0.42
1:C:173:SER:O	1:C:174:ARG:C	2.60	0.42
1:C:365:THR:O	1:C:369:ARG:HB2	2.20	0.42
1:D:120:PRO:HB3	1:D:179:TYR:CD2	2.54	0.42
1:D:167:ILE:HG22	1:D:171:LYS:HD2	2.02	0.42
1:A:405:THR:HG23	1:A:406:PRO:HD2	2.01	0.42
1:C:13:LEU:HD22	1:C:401:GLN:HE21	1.85	0.42
1:D:368:LEU:HD21	1:D:383:LEU:HB3	2.01	0.42
1:B:225:ASN:OD1	1:B:226:PRO:HD2	2.19	0.41
1:B:225:ASN:ND2	1:B:228:HIS:CE1	2.88	0.41
1:B:297:ARG:O	1:B:305:HIS:HB2	2.20	0.41
1:D:106:TYR:CD1	1:D:106:TYR:N	2.88	0.41
1:D:139:PHE:O	1:D:190:MET:HA	2.20	0.41
1:B:17:TRP:CH2	1:B:31:VAL:HG23	2.55	0.41
1:C:46:HIS:NE2	1:C:335:PHE:O	2.53	0.41
1:C:116:ASP:C	1:C:117:GLN:HG2	2.39	0.41
1:C:193:TRP:CZ2	2:C:3462:RNS:H11	2.55	0.41
1:A:156:SER:OG	1:A:196:ASP:OD2	2.36	0.41
1:B:393:GLN:HG2	1:C:389:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ILE:HG12	5:C:3544:HOH:O	2.21	0.41
1:D:225:ASN:O	1:D:228:HIS:N	2.38	0.41
1:B:33:GLU:OE1	1:B:36:ARG:NE	2.52	0.41
1:B:216:LEU:O	1:B:220:ILE:HG12	2.19	0.41
1:C:398:MET:CE	1:C:402:ARG:CG	2.98	0.41
1:C:405:THR:HG23	1:C:406:PRO:HD2	2.02	0.41
1:D:252:PHE:CD2	1:D:252:PHE:C	2.99	0.41
1:B:71:GLY:HA3	1:B:339:SER:CA	2.51	0.41
1:B:71:GLY:HA3	1:B:339:SER:HA	2.03	0.41
1:B:113:VAL:O	1:B:114:SER:C	2.58	0.41
1:C:121:GLU:HB3	5:C:3672:HOH:O	2.19	0.41
1:C:125:ASN:HA	1:C:128:GLU:HG3	2.02	0.41
1:C:271:PHE:HB3	1:C:275:GLU:OE1	2.20	0.41
1:C:114:SER:OG	1:C:116:ASP:OD1	2.37	0.41
1:D:95:PRO:HD3	1:D:405:THR:HG21	2.02	0.41
1:A:293:LEU:HD12	1:A:329:VAL:CG1	2.50	0.41
1:B:37:GLN:OE1	1:B:37:GLN:HA	2.21	0.41
1:B:95:PRO:HD3	1:B:405:THR:HG21	2.02	0.41
1:C:13:LEU:HD22	1:C:401:GLN:NE2	2.36	0.41
1:A:86:ASP:OD1	1:A:418:TYR:OH	2.30	0.41
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.90	0.41
1:B:124:LYS:HD3	1:B:179:TYR:OH	2.21	0.41
1:B:369:ARG:HD2	5:B:2714:HOH:O	2.20	0.41
1:C:137:LEU:HD23	1:C:137:LEU:HA	1.95	0.41
1:C:314:GLN:HE22	1:C:356:ALA:HA	1.86	0.41
1:D:179:TYR:CE1	1:D:183:GLN:HG3	2.56	0.41
1:A:194:ILE:HD12	1:A:196:ASP:CG	2.46	0.40
1:B:11:THR:O	1:B:15:GLN:HG3	2.21	0.40
1:B:83:LEU:HA	1:B:83:LEU:HD12	1.81	0.40
1:B:295:VAL:HG12	1:B:307:VAL:HG22	1.98	0.40
1:C:195:PRO:O	1:C:196:ASP:C	2.62	0.40
1:C:314:GLN:NE2	1:C:356:ALA:HA	2.36	0.40
1:D:267:ASP:HA	1:D:294:HIS:HB2	2.03	0.40
1:A:393:GLN:HG2	1:D:389:SER:O	2.21	0.40
1:A:424:SER:OG	1:A:425:ARG:HG2	2.21	0.40
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.88	0.40
1:B:410:GLU:O	1:B:411:TRP:C	2.64	0.40
1:A:46:HIS:NE2	1:A:335:PHE:O	2.54	0.40
1:A:335:PHE:C	1:A:335:PHE:CD1	2.99	0.40
1:A:390:LEU:HD23	1:A:390:LEU:HA	1.76	0.40
1:B:19:LEU:HD23	1:B:19:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:HD23	1:B:390:LEU:HA	1.96	0.40
1:D:314:GLN:NE2	1:D:356:ALA:HA	2.37	0.40
1:D:418:TYR:HA	1:D:421:GLU:HG2	2.02	0.40
1:A:151:ASP:HB2	5:A:1598:HOH:O	2.20	0.40
1:B:13:LEU:HD21	1:B:398:MET:HA	2.04	0.40
1:B:111:THR:HA	1:B:112:PRO:HD3	1.88	0.40
1:B:178:ALA:HA	1:B:229:HIS:HB2	2.03	0.40
1:B:314:GLN:NE2	1:B:359:ARG:HD3	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	414/426 (97%)	397 (96%)	15 (4%)	2 (0%)	24	22
1	B	414/426 (97%)	397 (96%)	14 (3%)	3 (1%)	18	15
1	C	414/426 (97%)	394 (95%)	17 (4%)	3 (1%)	18	15
1	D	414/426 (97%)	395 (95%)	17 (4%)	2 (0%)	24	22
All	All	1656/1704 (97%)	1583 (96%)	63 (4%)	10 (1%)	21	18

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	B	62	SER
1	C	62	SER
1	D	62	SER
1	C	59	PRO
1	D	59	PRO
1	B	53	VAL

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Mol	Chain	Res	Type
1	C	61	GLY
1	A	61	GLY
1	B	61	GLY

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	351/359 (98%)	332 (95%)	19 (5%)	20	18
1	B	351/359 (98%)	330 (94%)	21 (6%)	17	15
1	C	351/359 (98%)	329 (94%)	22 (6%)	16	14
1	D	351/359 (98%)	326 (93%)	25 (7%)	13	11
All	All	1404/1436 (98%)	1317 (94%)	87 (6%)	16	14

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	53	VAL
1	A	63	LEU
1	A	79	ASN
1	A	98	LYS
1	A	103	HIS
1	A	134	GLN
1	A	140	ASN
1	A	188	SER
1	A	223	LYS
1	A	290	GLN
1	A	324	ASP
1	A	336	PHE
1	A	343	ILE
1	A	369	ARG
1	A	374	PRO
1	A	383	LEU
1	A	401	GLN

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Mol	Chain	Res	Type
1	A	410	GLU
1	B	11	THR
1	B	27	VAL
1	B	53	VAL
1	B	63	LEU
1	B	79	ASN
1	B	98	LYS
1	B	103	HIS
1	B	119	LYS
1	B	128	GLU
1	B	134	GLN
1	B	140	ASN
1	B	171	LYS
1	B	188	SER
1	B	223	LYS
1	B	290	GLN
1	B	324	ASP
1	B	336	PHE
1	B	369	ARG
1	B	374	PRO
1	B	383	LEU
1	B	401	GLN
1	C	27	VAL
1	C	53	VAL
1	C	63	LEU
1	C	79	ASN
1	C	89	GLN
1	C	98	LYS
1	C	103	HIS
1	C	117	GLN
1	C	119	LYS
1	C	128	GLU
1	C	134	GLN
1	C	140	ASN
1	C	188	SER
1	C	223	LYS
1	C	290	GLN
1	C	324	ASP
1	C	336	PHE
1	C	369	ARG
1	C	374	PRO
1	C	383	LEU

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Mol	Chain	Res	Type
1	C	401	GLN
1	C	410	GLU
1	D	11	THR
1	D	27	VAL
1	D	53	VAL
1	D	57	GLU
1	D	63	LEU
1	D	79	ASN
1	D	89	GLN
1	D	98	LYS
1	D	103	HIS
1	D	117	GLN
1	D	128	GLU
1	D	134	GLN
1	D	140	ASN
1	D	173	SER
1	D	196	ASP
1	D	223	LYS
1	D	290	GLN
1	D	324	ASP
1	D	336	PHE
1	D	369	ARG
1	D	374	PRO
1	D	383	LEU
1	D	401	GLN
1	D	410	GLU
1	D	425	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	79	ASN
1	A	122	HIS
1	A	125	ASN
1	A	134	GLN
1	A	169	HIS
1	A	191	ASN
1	A	314	GLN
1	A	393	GLN
1	B	49	GLN
1	B	72	ASN

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Mol	Chain	Res	Type
1	B	79	ASN
1	B	122	HIS
1	B	125	ASN
1	B	134	GLN
1	B	169	HIS
1	B	228	HIS
1	B	314	GLN
1	C	49	GLN
1	C	58	ASN
1	C	79	ASN
1	C	122	HIS
1	C	125	ASN
1	C	134	GLN
1	C	140	ASN
1	C	169	HIS
1	C	314	GLN
1	C	387	GLN
1	C	393	GLN
1	D	49	GLN
1	D	79	ASN
1	D	122	HIS
1	D	125	ASN
1	D	134	GLN
1	D	169	HIS
1	D	314	GLN
1	D	387	GLN

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	RNS	B	2462	-	9,10,10	1.24	2 (22%)	12,13,13	1.21	1 (8%)
2	RNS	C	3462	-	9,10,10	1.13	1 (11%)	12,13,13	1.05	1 (8%)
2	RNS	D	4462	-	9,10,10	0.97	0	12,13,13	0.93	0
2	RNS	A	1462	4	9,10,10	1.05	1 (11%)	12,13,13	1.78	4 (33%)

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	RNS	B	2462	-	-	5/13/14/14	-
2	RNS	C	3462	-	-	7/13/14/14	-
2	RNS	D	4462	-	-	8/13/14/14	-
2	RNS	A	1462	4	-	5/13/14/14	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3462	RNS	O5-C5	2.64	1.50	1.43
2	B	2462	RNS	O5-C5	2.19	1.48	1.43
2	A	1462	RNS	O5-C5	2.08	1.48	1.43
2	B	2462	RNS	O3-C3	2.04	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1462	RNS	O3-C3-C2	3.36	115.38	109.13
2	A	1462	RNS	O3-C3-C4	2.73	115.83	109.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2462	RNS	C4-C3-C2	-2.68	108.79	113.49
2	C	3462	RNS	C4-C3-C2	-2.43	109.23	113.49
2	A	1462	RNS	O4-C4-C5	2.31	113.53	109.14
2	A	1462	RNS	C3-C2-C1	-2.16	104.45	111.03

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1462	RNS	C3-C4-C5-O5
2	B	2462	RNS	C3-C4-C5-C6
2	B	2462	RNS	C3-C4-C5-O5
2	B	2462	RNS	O4-C4-C5-O5
2	C	3462	RNS	C3-C4-C5-C6
2	C	3462	RNS	C3-C4-C5-O5
2	C	3462	RNS	O4-C4-C5-O5
2	D	4462	RNS	C3-C4-C5-O5
2	D	4462	RNS	O4-C4-C5-O5
2	A	1462	RNS	O3-C3-C4-O4
2	C	3462	RNS	O3-C3-C4-O4
2	B	2462	RNS	O4-C4-C5-C6
2	C	3462	RNS	C2-C3-C4-O4
2	C	3462	RNS	O4-C4-C5-C6
2	C	3462	RNS	O3-C3-C4-C5
2	A	1462	RNS	O4-C4-C5-O5
2	D	4462	RNS	O2-C2-C3-O3
2	D	4462	RNS	C3-C4-C5-C6
2	D	4462	RNS	O2-C2-C3-C4
2	D	4462	RNS	O4-C4-C5-C6
2	D	4462	RNS	C2-C3-C4-O4
2	A	1462	RNS	O3-C3-C4-C5
2	B	2462	RNS	O3-C3-C4-O4
2	A	1462	RNS	C3-C4-C5-C6
2	D	4462	RNS	O3-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3462	RNS	2	0
2	A	1462	RNS	4	0

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

6.1 Protein, DNA and RNA chains

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	416/426 (97%)	-0.22	17 (4%) 41 43	15, 26, 52, 79	15 (3%)
1	B	416/426 (97%)	-0.36	18 (4%) 40 41	14, 23, 48, 76	15 (3%)
1	C	416/426 (97%)	-0.31	16 (3%) 44 46	15, 24, 50, 78	15 (3%)
1	D	416/426 (97%)	-0.19	19 (4%) 37 39	16, 27, 52, 80	15 (3%)
All	All	1664/1704 (97%)	-0.27	70 (4%) 40 42	14, 25, 51, 80	60 (3%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	59	PRO	6.2
1	A	69	ALA	5.9
1	A	67	ILE	5.9
1	B	67	ILE	5.7
1	D	61	GLY	5.6
1	C	59	PRO	5.6
1	C	61	GLY	5.2
1	B	72	ASN	5.0
1	C	69	ALA	5.0
1	B	59	PRO	5.0
1	A	61	GLY	4.8
1	D	59	PRO	4.8
1	A	336	PHE	4.6
1	B	336	PHE	4.6
1	C	336	PHE	4.5
1	D	58	ASN	4.5
1	C	67	ILE	4.4
1	D	69	ALA	4.4
1	D	60	GLU	4.2
1	D	336	PHE	4.2
1	B	61	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	64	THR	4.2
1	B	69	ALA	4.1
1	D	67	ILE	4.1
1	C	60	GLU	4.1
1	C	63	LEU	4.0
1	B	63	LEU	4.0
1	D	62	SER	3.9
1	D	72	ASN	3.9
1	C	72	ASN	3.9
1	A	63	LEU	3.8
1	C	71	GLY	3.8
1	A	58	ASN	3.8
1	D	63	LEU	3.8
1	D	64	THR	3.8
1	B	64	THR	3.7
1	A	64	THR	3.6
1	A	60	GLU	3.5
1	C	68	GLN	3.2
1	B	65	GLY	3.2
1	D	65	GLY	3.1
1	C	58	ASN	3.0
1	C	70	THR	2.9
1	A	68	GLN	2.9
1	A	65	GLY	2.9
1	C	65	GLY	2.9
1	B	58	ASN	2.8
1	D	68	GLN	2.8
1	A	11	THR	2.8
1	B	71	GLY	2.7
1	A	72	ASN	2.6
1	D	421	GLU	2.6
1	B	11	THR	2.6
1	C	11	THR	2.6
1	A	71	GLY	2.6
1	D	425	ARG	2.5
1	D	71	GLY	2.4
1	D	27	VAL	2.3
1	B	70	THR	2.3
1	A	62	SER	2.2
1	C	66	GLY	2.2
1	B	421	GLU	2.2
1	B	68	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	70	THR	2.2
1	B	425	ARG	2.1
1	A	424	SER	2.1
1	D	11	THR	2.1
1	B	62	SER	2.1
1	A	401	GLN	2.1
1	B	60	GLU	2.0

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	RNS	B	2462	11/11	0.85	0.19	13,24,42,56	11
2	RNS	C	3462	11/11	0.85	0.23	11,25,38,45	11
2	RNS	D	4462	11/11	0.85	0.18	4,19,30,37	11
2	RNS	A	1462	11/11	0.87	0.13	9,19,30,36	11
4	MN	D	451	1/1	0.91	0.09	60,60,60,60	0
4	MN	A	451	1/1	0.93	0.08	59,59,59,59	0
4	MN	C	451	1/1	0.95	0.07	51,51,51,51	0
4	MN	B	451	1/1	0.96	0.07	53,53,53,53	0
3	ZN	C	450	1/1	0.98	0.04	36,36,36,36	0
3	ZN	D	450	1/1	0.98	0.04	41,41,41,41	0
3	ZN	B	450	1/1	0.98	0.03	34,34,34,34	0
3	ZN	A	450	1/1	0.99	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.