



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:36 PM UTC

PDB ID : 1QMI / pdb_00001qmi
Title : Crystal structure of RNA 3'-terminal phosphate cyclase, an ubiquitous enzyme with unusual topology
Authors : Palm, G.J.; Billy, E.; Filipowicz, W.; Wlodawer, A.
Deposited on : 1999-09-28
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

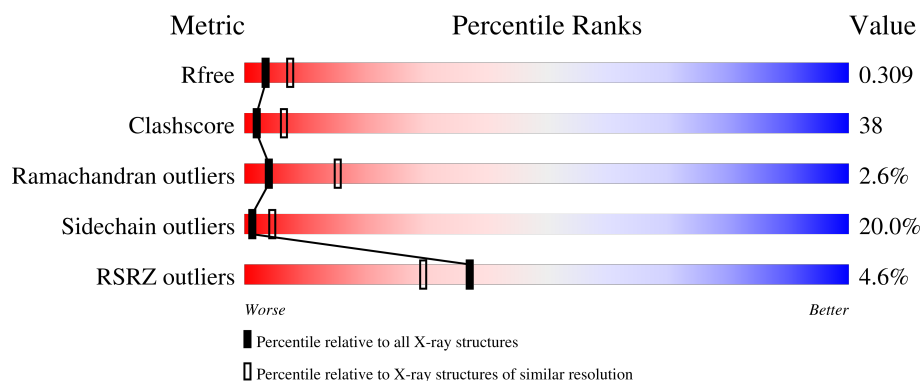
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	347	4% 35% 44% 14% . .
1	B	347	4% 35% 46% 14% . .
1	C	347	4% 35% 44% 15% . .
1	D	347	5% 37% 46% 11% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9972 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 RNA 3'-TERMINAL PHOSPHATE CYCLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	Se	0	0	0
			2493	1571	449	466	3	4			
1	B	335	Total	C	N	O	S	Se	0	0	0
			2493	1571	449	466	3	4			
1	C	335	Total	C	N	O	S	Se	0	0	0
			2493	1571	449	466	3	4			
1	D	335	Total	C	N	O	S	Se	0	0	0
			2493	1571	449	466	3	4			

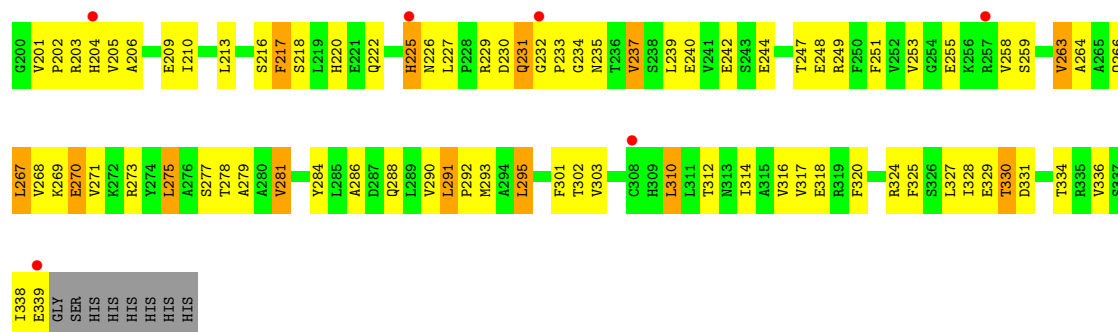
There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP P46849
A	2	VAL	-	expression tag	UNP P46849
A	340	GLY	-	expression tag	UNP P46849
A	341	SER	-	expression tag	UNP P46849
A	342	HIS	-	expression tag	UNP P46849
A	343	HIS	-	expression tag	UNP P46849
A	344	HIS	-	expression tag	UNP P46849
A	345	HIS	-	expression tag	UNP P46849
A	346	HIS	-	expression tag	UNP P46849
A	347	HIS	-	expression tag	UNP P46849
B	1	MSE	-	expression tag	UNP P46849
B	2	VAL	-	expression tag	UNP P46849
B	340	GLY	-	expression tag	UNP P46849
B	341	SER	-	expression tag	UNP P46849
B	342	HIS	-	expression tag	UNP P46849
B	343	HIS	-	expression tag	UNP P46849
B	344	HIS	-	expression tag	UNP P46849
B	345	HIS	-	expression tag	UNP P46849
B	346	HIS	-	expression tag	UNP P46849
B	347	HIS	-	expression tag	UNP P46849
C	1	MSE	-	expression tag	UNP P46849

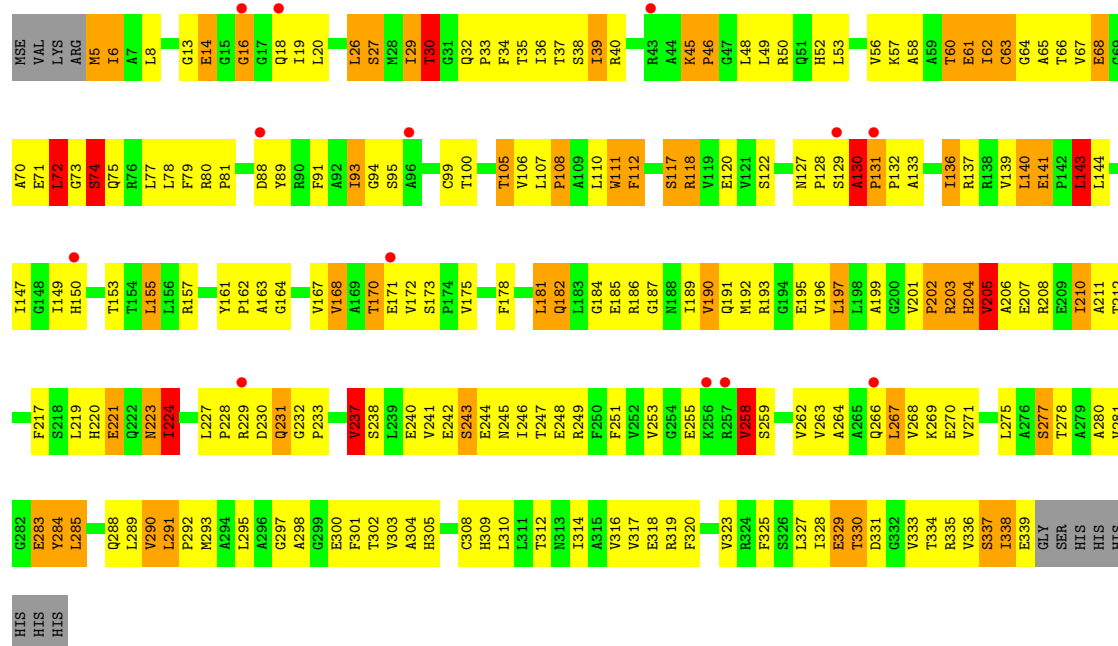
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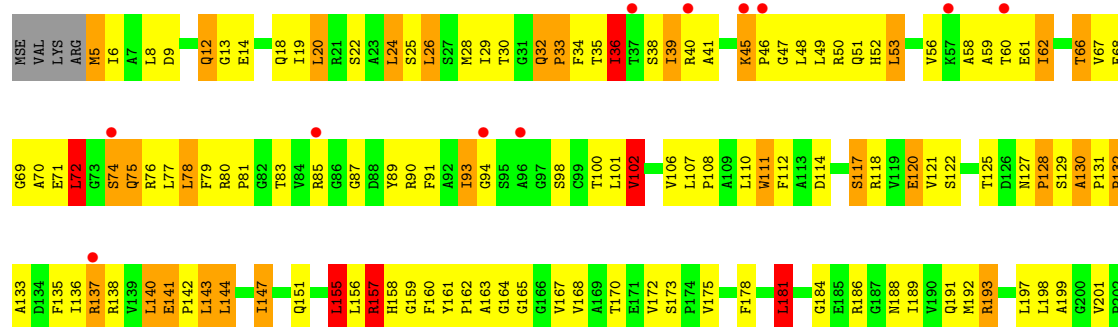
Chain	Residue	Modelled	Actual	Comment	Reference
C	2	VAL	-	expression tag	UNP P46849
C	340	GLY	-	expression tag	UNP P46849
C	341	SER	-	expression tag	UNP P46849
C	342	HIS	-	expression tag	UNP P46849
C	343	HIS	-	expression tag	UNP P46849
C	344	HIS	-	expression tag	UNP P46849
C	345	HIS	-	expression tag	UNP P46849
C	346	HIS	-	expression tag	UNP P46849
C	347	HIS	-	expression tag	UNP P46849
D	1	MSE	-	expression tag	UNP P46849
D	2	VAL	-	expression tag	UNP P46849
D	340	GLY	-	expression tag	UNP P46849
D	341	SER	-	expression tag	UNP P46849
D	342	HIS	-	expression tag	UNP P46849
D	343	HIS	-	expression tag	UNP P46849
D	344	HIS	-	expression tag	UNP P46849
D	345	HIS	-	expression tag	UNP P46849
D	346	HIS	-	expression tag	UNP P46849
D	347	HIS	-	expression tag	UNP P46849

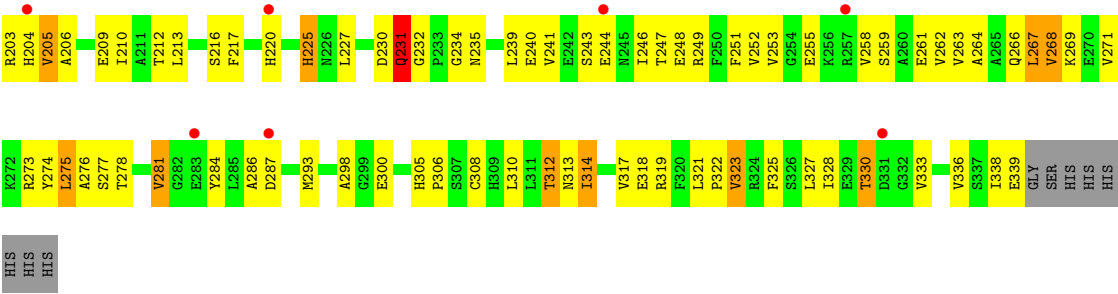


• Molecule 1: RNA 3'-TERMINAL PHOSPHATE CYCLASE



• Molecule 1: RNA 3'-TERMINAL PHOSPHATE CYCLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.80Å 126.60Å 128.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	89.8 (10.00-2.80) 90.2 (10.00-2.81)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.76 (at 2.79Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.244 , 0.331 0.221 , 0.309	Depositor DCC
R_{free} test set	1997 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9972	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6224e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.15	5/2533 (0.2%)	1.45	39/3436 (1.1%)
1	B	1.09	3/2533 (0.1%)	1.44	41/3436 (1.2%)
1	C	1.18	9/2533 (0.4%)	1.42	34/3436 (1.0%)
1	D	1.05	0/2533	1.43	31/3436 (0.9%)
All	All	1.12	17/10132 (0.2%)	1.43	145/13744 (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	A	0	1
1	C	0	1
All	All	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	VAL	CA-CB	8.97	1.66	1.54
1	A	271	VAL	CA-CB	-7.35	1.45	1.54
1	C	290	VAL	CA-CB	-7.06	1.46	1.54
1	A	141	GLU	CA-C	6.34	1.60	1.52
1	B	23	ALA	CA-CB	-6.31	1.43	1.53
1	A	223	ASN	CA-C	-5.80	1.45	1.52
1	C	237	VAL	CA-CB	5.74	1.61	1.54
1	C	190	VAL	CA-CB	-5.71	1.47	1.54
1	C	221	GLU	CA-C	-5.65	1.45	1.52
1	A	290	VAL	CA-CB	-5.49	1.48	1.54
1	C	241	VAL	CA-CB	-5.44	1.46	1.53
1	B	217	PHE	CA-C	-5.39	1.46	1.52
1	B	251	PHE	CA-C	-5.20	1.46	1.52
1	C	258	VAL	CA-CB	5.19	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	168	VAL	CA-CB	-5.11	1.48	1.54
1	C	60	THR	CA-CB	5.11	1.58	1.53
1	C	309	HIS	CA-C	-5.11	1.46	1.52

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	45	LYS	CA-C-N	15.47	139.18	119.84
1	D	45	LYS	C-N-CA	15.47	139.18	119.84
1	A	45	LYS	CA-C-N	12.44	135.38	119.84
1	A	45	LYS	C-N-CA	12.44	135.38	119.84
1	B	45	LYS	CA-C-N	10.71	133.22	119.84
1	B	45	LYS	C-N-CA	10.71	133.22	119.84
1	C	45	LYS	CA-C-N	9.82	132.12	119.84
1	C	45	LYS	C-N-CA	9.82	132.12	119.84
1	D	143	LEU	N-CA-C	-9.39	101.12	111.36
1	B	139	VAL	N-CA-C	9.15	118.85	111.62
1	A	139	VAL	N-CA-C	9.14	118.84	111.62
1	B	29	ILE	N-CA-C	-8.57	101.99	110.30
1	B	281	VAL	N-CA-C	8.45	122.06	108.97
1	D	281	VAL	N-CA-C	8.40	121.66	108.89
1	B	310	LEU	N-CA-C	-7.69	102.84	111.07
1	D	286	ALA	N-CA-C	-7.63	102.90	111.07
1	B	143	LEU	N-CA-C	-7.48	103.07	111.07
1	A	163	ALA	N-CA-C	7.45	119.09	110.97
1	A	62	ILE	N-CA-C	-7.31	101.95	111.09
1	D	106	VAL	N-CA-C	7.31	117.91	110.82
1	A	6	ILE	N-CA-C	7.29	119.21	109.37
1	B	330	THR	N-CA-C	7.19	120.60	108.02
1	D	61	GLU	N-CA-C	-7.19	106.42	114.62
1	B	155	LEU	N-CA-C	-7.14	97.61	109.46
1	B	30	THR	N-CA-C	7.12	119.12	111.36
1	A	164	GLY	N-CA-C	-7.02	101.57	112.45
1	B	127	ASN	CA-C-N	6.86	126.37	119.24
1	B	127	ASN	C-N-CA	6.86	126.37	119.24
1	B	102	VAL	N-CA-C	-6.80	103.90	110.42
1	C	143	LEU	N-CA-C	-6.80	103.95	111.36
1	C	285	LEU	N-CA-C	-6.73	103.95	111.28
1	D	155	LEU	N-CA-C	-6.73	100.32	110.28
1	A	102	VAL	N-CA-C	-6.71	104.22	110.53
1	C	29	ILE	N-CA-C	-6.66	104.03	110.42
1	A	202	PRO	N-CA-C	6.66	121.80	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	111	TRP	N-CA-C	-6.64	104.65	112.89
1	A	30	THR	N-CA-C	6.64	118.31	111.14
1	B	190	VAL	N-CA-C	-6.51	107.52	113.71
1	D	181	LEU	CA-CB-CG	6.47	138.96	116.30
1	A	29	ILE	N-CA-C	-6.44	103.53	110.23
1	B	266	GLN	N-CA-C	-6.41	104.37	111.36
1	D	137	ARG	N-CA-C	6.34	117.85	111.07
1	B	111	TRP	N-CA-C	-6.30	105.07	112.89
1	A	281	VAL	N-CA-C	6.28	118.78	108.99
1	A	106	VAL	N-CA-C	6.25	117.81	111.00
1	A	127	ASN	CA-C-N	6.24	125.72	119.24
1	A	127	ASN	C-N-CA	6.24	125.72	119.24
1	B	46	PRO	N-CA-C	6.23	125.31	112.47
1	B	106	VAL	N-CA-C	6.22	116.40	110.74
1	B	19	ILE	N-CA-C	-6.20	104.30	110.62
1	B	118	ARG	N-CA-C	-6.15	98.61	109.06
1	C	74	SER	N-CA-C	6.09	119.18	110.10
1	C	258	VAL	CB-CA-C	6.09	119.22	110.33
1	B	95	SER	N-CA-C	-6.08	105.77	113.43
1	C	163	ALA	N-CA-C	6.06	117.57	110.97
1	C	6	ILE	N-CA-C	6.05	117.53	109.37
1	C	164	GLY	N-CA-C	-6.04	101.83	112.77
1	B	36	ILE	N-CA-C	-6.04	99.69	108.87
1	C	204	HIS	N-CA-C	-6.03	106.25	113.97
1	D	102	VAL	N-CA-C	-5.96	104.70	110.42
1	A	87	GLY	N-CA-C	5.92	118.00	110.96
1	C	63	CYS	N-CA-C	5.91	117.99	110.61
1	B	286	ALA	N-CA-C	-5.90	104.76	111.07
1	C	131	PRO	CA-C-N	5.89	126.39	120.14
1	C	131	PRO	C-N-CA	5.89	126.39	120.14
1	C	127	ASN	CA-C-N	5.88	125.09	118.97
1	C	127	ASN	C-N-CA	5.88	125.09	118.97
1	D	120	GLU	N-CA-C	-5.88	98.70	108.34
1	D	74	SER	N-CA-C	5.88	118.75	110.23
1	C	330	THR	N-CA-C	5.87	118.38	107.99
1	D	205	VAL	N-CA-C	-5.85	104.63	111.00
1	A	285	LEU	N-CA-C	-5.80	105.09	111.82
1	A	227	LEU	CA-C-N	5.79	125.79	119.89
1	A	227	LEU	C-N-CA	5.79	125.79	119.89
1	B	46	PRO	CA-C-N	-5.78	117.71	122.16
1	B	46	PRO	C-N-CA	-5.78	117.71	122.16
1	C	328	ILE	N-CA-CB	-5.75	106.90	112.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	GLN	N-CA-C	-5.74	105.61	113.30
1	D	204	HIS	N-CA-C	-5.73	106.63	113.97
1	A	55	ALA	N-CA-C	-5.71	104.96	111.07
1	A	99	CYS	N-CA-C	-5.62	105.15	111.28
1	D	227	LEU	N-CA-C	-5.62	101.96	110.50
1	C	281	VAL	N-CA-C	5.61	117.90	109.20
1	C	62	ILE	CB-CA-C	-5.60	103.48	112.16
1	C	224	ILE	N-CA-C	-5.58	100.30	108.11
1	B	229	ARG	CA-C-N	5.57	128.02	120.38
1	B	229	ARG	C-N-CA	5.57	128.02	120.38
1	A	63	CYS	N-CA-C	5.57	119.87	112.30
1	C	202	PRO	N-CA-C	5.55	120.20	111.38
1	D	330	THR	N-CA-C	5.52	118.50	107.62
1	A	181	LEU	CA-CB-CG	5.52	135.62	116.30
1	D	78	LEU	N-CA-C	-5.51	98.93	108.69
1	D	199	ALA	N-CA-C	-5.51	96.80	107.44
1	D	36	ILE	N-CA-C	-5.51	100.50	108.71
1	A	259	SER	N-CA-C	5.43	118.51	110.48
1	D	157	ARG	N-CA-C	-5.38	99.83	108.55
1	B	204	HIS	N-CA-C	-5.37	107.09	113.97
1	A	131	PRO	CA-C-N	5.37	125.83	120.14
1	A	131	PRO	C-N-CA	5.37	125.83	120.14
1	A	95	SER	N-CA-C	-5.33	106.71	113.43
1	A	330	THR	N-CA-C	5.33	117.42	107.99
1	D	244	GLU	N-CA-C	5.32	116.93	111.03
1	D	75	GLN	N-CA-C	-5.32	106.17	113.30
1	B	63	CYS	N-CA-C	5.30	119.30	112.41
1	D	138	ARG	N-CA-C	5.27	119.56	113.18
1	B	53	LEU	N-CA-C	-5.27	105.61	111.36
1	C	205	VAL	N-CA-C	-5.26	105.26	111.00
1	D	62	ILE	N-CA-C	-5.26	104.52	111.09
1	B	164	GLY	N-CA-C	-5.26	104.30	112.45
1	C	95	SER	N-CA-C	-5.25	106.81	113.43
1	C	130	ALA	CA-C-N	5.24	125.78	120.38
1	C	130	ALA	C-N-CA	5.24	125.78	120.38
1	C	30	THR	N-CA-C	5.22	116.78	111.14
1	A	115	GLY	CA-C-N	5.22	125.51	119.92
1	A	115	GLY	C-N-CA	5.22	125.51	119.92
1	C	309	HIS	N-CA-C	-5.22	105.27	111.69
1	A	149	ILE	CA-C-N	-5.22	115.25	123.13
1	A	149	ILE	C-N-CA	-5.22	115.25	123.13
1	D	118	ARG	N-CA-C	-5.20	99.49	108.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	HIS	N-CA-C	5.19	118.12	107.69
1	B	115	GLY	CA-C-N	5.18	125.16	120.03
1	B	115	GLY	C-N-CA	5.18	125.16	120.03
1	B	295	LEU	N-CA-C	-5.16	105.84	111.82
1	B	39	ILE	CA-C-N	-5.13	113.43	123.13
1	B	39	ILE	C-N-CA	-5.13	113.43	123.13
1	D	164	GLY	N-CA-C	-5.12	103.50	112.77
1	A	36	ILE	N-CA-C	-5.11	101.10	108.87
1	C	150	HIS	N-CA-C	5.10	117.01	107.99
1	C	37	THR	N-CA-C	5.08	120.13	113.88
1	C	181	LEU	CA-CB-CG	5.08	134.08	116.30
1	C	187	GLY	N-CA-C	-5.08	104.20	112.83
1	B	72	LEU	N-CA-C	5.07	121.61	110.80
1	B	163	ALA	N-CA-C	5.07	116.50	110.97
1	B	137	ARG	N-CA-C	5.07	116.61	111.14
1	A	205	VAL	CB-CA-C	-5.06	105.46	112.24
1	C	111	TRP	N-CA-C	-5.05	106.37	112.54
1	D	33	PRO	N-CA-C	-5.04	103.62	111.13
1	A	20	LEU	CA-CB-CG	5.04	133.92	116.30
1	D	163	ALA	N-CA-C	5.03	116.45	110.97
1	A	82	GLY	N-CA-C	-5.02	102.32	111.16
1	A	29	ILE	CB-CA-C	-5.02	105.28	111.70
1	D	159	GLY	N-CA-C	-5.02	101.29	113.18
1	C	139	VAL	N-CA-C	5.01	119.76	109.34
1	B	263	VAL	N-CA-C	-5.01	105.02	110.23
1	A	33	PRO	N-CA-C	-5.00	103.67	111.13

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	TYR	Sidechain
1	C	284	TYR	Sidechain

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	2493	0	2533	196	0
1	B	2493	0	2533	201	0
1	C	2493	0	2533	208	0
1	D	2493	0	2533	165	0
All	All	9972	0	10132	764	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 38.

All (764) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:MSE:HE2	1:B:33:PRO:HB2	1.32	1.11
1:D:293:MSE:HB3	1:D:338:ILE:HD11	1.30	1.10
1:D:239:LEU:HD13	1:D:271:VAL:HG21	1.26	1.07
1:D:26:LEU:O	1:D:30:THR:HG22	1.55	1.05
1:B:26:LEU:O	1:B:30:THR:HG22	1.62	0.97
1:A:90:ARG:HG2	1:A:90:ARG:HH11	1.30	0.95
1:C:237:VAL:HG22	1:C:267:LEU:HD12	1.46	0.94
1:D:192:MSE:HE1	1:D:275:LEU:HD21	1.48	0.94
1:C:60:THR:HG22	1:C:79:PHE:HE1	1.31	0.94
1:A:60:THR:HG22	1:A:79:PHE:HE1	1.34	0.93
1:A:29:ILE:HD12	1:A:112:PHE:CE2	2.04	0.93
1:A:56:VAL:O	1:A:60:THR:HG23	1.69	0.92
1:C:34:PHE:CE1	1:C:79:PHE:HB3	2.05	0.92
1:D:205:VAL:O	1:D:209:GLU:HG3	1.70	0.91
1:A:327:LEU:CD2	1:A:336:VAL:HG22	2.02	0.90
1:C:329:GLU:HB2	1:D:327:LEU:H	1.37	0.89
1:C:197:LEU:HD21	1:C:227:LEU:HG	1.53	0.89
1:B:213:LEU:HD22	1:B:239:LEU:HD12	1.55	0.89
1:B:197:LEU:HD23	1:B:225:HIS:HB3	1.53	0.87
1:C:30:THR:HG23	1:C:32:GLN:H	1.38	0.87
1:B:205:VAL:O	1:B:209:GLU:HG3	1.75	0.87
1:B:217:PHE:HE2	1:B:268:VAL:HG13	1.37	0.86
1:B:45:LYS:HE2	1:B:45:LYS:HA	1.57	0.86
1:B:184:GLY:HA2	1:B:302:THR:HG23	1.57	0.86
1:C:93:ILE:HG13	1:C:122:SER:O	1.75	0.85
1:D:58:ALA:O	1:D:62:ILE:HG12	1.77	0.85
1:D:175:VAL:HG11	1:D:178:PHE:CE2	2.12	0.84
1:A:5:MSE:HG3	1:A:33:PRO:HG2	1.59	0.84
1:B:29:ILE:HD12	1:B:112:PHE:CD2	2.13	0.83
1:A:29:ILE:HD12	1:A:112:PHE:CD2	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:SER:HB3	1:B:101:LEU:HD12	1.60	0.83
1:C:40:ARG:NH2	1:C:49:LEU:HD11	1.94	0.83
1:A:264:ALA:O	1:A:268:VAL:HG23	1.77	0.83
1:B:291:LEU:HB3	1:B:292:PRO:HD3	1.61	0.82
1:C:56:VAL:O	1:C:60:THR:HG23	1.80	0.81
1:C:221:GLU:HB3	1:C:223:ASN:HD21	1.44	0.81
1:A:156:LEU:HB2	1:A:167:VAL:HG12	1.61	0.81
1:A:26:LEU:HD23	1:A:316:VAL:HG12	1.63	0.81
1:C:40:ARG:HD3	1:C:52:HIS:HE1	1.46	0.81
1:A:25:SER:O	1:A:29:ILE:HG12	1.81	0.81
1:C:155:LEU:CD1	1:C:168:VAL:HG22	2.10	0.81
1:D:62:ILE:HD11	1:D:91:PHE:HZ	1.46	0.81
1:C:60:THR:HG22	1:C:79:PHE:CE1	2.14	0.80
1:A:39:ILE:HD12	1:A:48:LEU:HG	1.62	0.80
1:C:255:GLU:HB2	1:C:258:VAL:HB	1.63	0.80
1:D:5:MSE:HE2	1:D:33:PRO:HB2	1.63	0.80
1:A:5:MSE:HE1	1:A:78:LEU:HD11	1.63	0.80
1:D:198:LEU:HD11	1:D:206:ALA:HB2	1.62	0.80
1:D:98:SER:HB3	1:D:101:LEU:HD12	1.63	0.80
1:B:48:LEU:HD11	1:B:77:LEU:HD13	1.64	0.79
1:A:29:ILE:HG23	1:A:112:PHE:CE2	2.17	0.79
1:A:93:ILE:HG12	1:A:122:SER:O	1.82	0.79
1:C:202:PRO:O	1:C:205:VAL:HG23	1.82	0.79
1:D:172:VAL:HG12	1:D:173:SER:H	1.47	0.78
1:A:45:LYS:HE2	1:A:45:LYS:HA	1.65	0.78
1:B:158:HIS:HB2	1:B:231:GLN:HG2	1.64	0.78
1:C:186:ARG:NH2	1:C:277:SER:O	2.18	0.77
1:B:40:ARG:NH2	1:B:45:LYS:HB2	2.00	0.77
1:C:34:PHE:CE2	1:C:36:ILE:HD11	2.20	0.77
1:B:217:PHE:CE2	1:B:268:VAL:HG13	2.20	0.76
1:B:38:SER:HA	1:B:75:GLN:HG2	1.66	0.76
1:C:131:PRO:HG3	1:C:284:TYR:CZ	2.21	0.76
1:A:68:GLU:HB2	1:A:78:LEU:HB3	1.68	0.75
1:A:26:LEU:O	1:A:30:THR:HG23	1.87	0.74
1:B:327:LEU:HD22	1:B:336:VAL:HG22	1.69	0.74
1:D:158:HIS:HB2	1:D:231:GLN:HG2	1.70	0.74
1:D:172:VAL:HG12	1:D:173:SER:N	2.01	0.74
1:C:48:LEU:HD12	1:C:74:SER:HB3	1.69	0.74
1:B:314:ILE:O	1:B:318:GLU:HG3	1.88	0.74
1:A:36:ILE:CG2	1:A:39:ILE:HG12	2.19	0.73
1:B:136:ILE:HA	1:B:140:LEU:HD22	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LEU:HD11	1:D:77:LEU:HD13	1.69	0.73
1:A:327:LEU:HD23	1:A:336:VAL:HG22	1.68	0.73
1:D:271:VAL:HG12	1:D:275:LEU:HD22	1.71	0.73
1:B:267:LEU:O	1:B:271:VAL:HG23	1.88	0.73
1:D:314:ILE:HG23	1:D:325:PHE:CD1	2.24	0.73
1:C:107:LEU:CD1	1:C:170:THR:HG21	2.18	0.72
1:A:186:ARG:NH2	1:A:277:SER:O	2.22	0.72
1:B:190:VAL:O	1:B:191:GLN:HB3	1.88	0.72
1:A:46:PRO:HB2	1:A:75:GLN:HE21	1.55	0.72
1:A:289:LEU:O	1:A:293:MSE:HG3	1.89	0.72
1:C:16:GLY:N	1:C:19:ILE:HD12	2.05	0.72
1:C:16:GLY:H	1:C:19:ILE:HD12	1.54	0.72
1:C:197:LEU:HD21	1:C:227:LEU:CG	2.20	0.72
1:A:294:ALA:HA	1:A:338:ILE:HD11	1.70	0.71
1:B:239:LEU:HD13	1:B:271:VAL:HG21	1.72	0.71
1:A:265:ALA:O	1:A:269:LYS:HG3	1.90	0.71
1:B:56:VAL:O	1:B:60:THR:HG23	1.91	0.71
1:A:36:ILE:HG21	1:A:39:ILE:HG12	1.71	0.71
1:B:158:HIS:H	1:B:231:GLN:HE21	1.38	0.71
1:C:107:LEU:HD11	1:C:170:THR:HG21	1.72	0.71
1:C:155:LEU:HD11	1:C:168:VAL:HG22	1.73	0.71
1:D:40:ARG:HD2	1:D:52:HIS:HE1	1.55	0.70
1:D:66:THR:HB	1:D:80:ARG:HB2	1.73	0.70
1:A:60:THR:HG22	1:A:79:PHE:CE1	2.22	0.70
1:D:258:VAL:HG12	1:D:263:VAL:HG23	1.73	0.70
1:C:58:ALA:O	1:C:62:ILE:HG12	1.91	0.70
1:D:6:ILE:HD11	1:D:32:GLN:HE21	1.55	0.70
1:B:328:ILE:HG22	1:B:330:THR:HG23	1.73	0.70
1:B:5:MSE:HE1	1:B:78:LEU:HD11	1.72	0.70
1:D:181:LEU:HD12	1:D:293:MSE:SE	2.41	0.70
1:B:44:ALA:O	1:B:46:PRO:HD3	1.92	0.70
1:C:197:LEU:CD2	1:C:227:LEU:HG	2.21	0.70
1:B:21:ARG:HB3	1:B:105:THR:HG23	1.74	0.70
1:A:16:GLY:HA2	1:A:19:ILE:HG13	1.72	0.70
1:D:34:PHE:HE1	1:D:36:ILE:HG12	1.57	0.70
1:A:5:MSE:HE1	1:A:78:LEU:CD1	2.20	0.70
1:A:35:THR:OG1	1:A:78:LEU:HD12	1.91	0.69
1:D:45:LYS:HE2	1:D:45:LYS:HA	1.73	0.69
1:B:40:ARG:HH22	1:B:49:LEU:HG	1.58	0.69
1:C:155:LEU:HD13	1:C:168:VAL:HG22	1.75	0.69
1:D:6:ILE:HD11	1:D:32:GLN:NE2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:VAL:HG12	1:C:263:VAL:HG22	1.74	0.69
1:D:128:PRO:HA	1:D:253:VAL:HB	1.75	0.69
1:D:25:SER:O	1:D:29:ILE:HG13	1.93	0.68
1:D:327:LEU:HD22	1:D:336:VAL:HG22	1.76	0.68
1:A:338:ILE:HG23	1:A:339:GLU:N	2.09	0.68
1:C:191:GLN:HE21	1:C:193:ARG:HD2	1.57	0.68
1:D:62:ILE:HD11	1:D:91:PHE:CZ	2.27	0.68
1:A:93:ILE:HD11	1:A:121:VAL:CG1	2.24	0.68
1:C:204:HIS:O	1:C:208:ARG:HG3	1.93	0.68
1:C:40:ARG:HH22	1:C:45:LYS:HB2	1.58	0.68
1:A:313:ASN:O	1:A:317:VAL:HG23	1.94	0.67
1:B:128:PRO:HA	1:B:253:VAL:HB	1.76	0.67
1:B:269:LYS:O	1:B:273:ARG:HG3	1.93	0.67
1:C:5:MSE:HE1	1:C:78:LEU:HD11	1.76	0.67
1:D:68:GLU:HB3	1:D:78:LEU:HB3	1.76	0.67
1:B:13:GLY:HA3	1:B:312:THR:CG2	2.25	0.66
1:B:60:THR:HG21	1:B:67:VAL:HG21	1.77	0.66
1:C:40:ARG:NH2	1:C:45:LYS:HB2	2.10	0.66
1:D:13:GLY:HA3	1:D:312:THR:CG2	2.25	0.66
1:D:217:PHE:HE2	1:D:268:VAL:HG22	1.60	0.66
1:C:13:GLY:HA3	1:C:312:THR:HG21	1.77	0.66
1:C:66:THR:HB	1:C:80:ARG:HB2	1.78	0.66
1:C:271:VAL:O	1:C:275:LEU:HD23	1.95	0.66
1:D:56:VAL:O	1:D:60:THR:HG23	1.96	0.66
1:B:196:VAL:HG11	1:B:206:ALA:HA	1.76	0.66
1:B:213:LEU:HD21	1:B:267:LEU:HD13	1.78	0.66
1:B:184:GLY:HA2	1:B:302:THR:CG2	2.25	0.66
1:C:258:VAL:HG12	1:C:263:VAL:CG2	2.26	0.66
1:C:327:LEU:CD2	1:C:336:VAL:HG22	2.25	0.66
1:B:36:ILE:HB	1:B:39:ILE:HD11	1.77	0.65
1:B:16:GLY:H	1:B:19:ILE:HD11	1.61	0.65
1:A:48:LEU:HB3	1:A:53:LEU:CD1	2.27	0.65
1:B:193:ARG:NH1	1:B:193:ARG:HG2	2.09	0.65
1:B:329:GLU:HG3	1:B:334:THR:OG1	1.96	0.65
1:A:141:GLU:HB3	1:A:142:PRO:HD3	1.77	0.65
1:B:293:MSE:HB3	1:B:338:ILE:HD12	1.79	0.65
1:C:230:ASP:C	1:C:232:GLY:H	2.04	0.65
1:D:85:ARG:HA	1:D:114:ASP:OD1	1.97	0.65
1:B:45:LYS:HE2	1:B:45:LYS:CA	2.27	0.65
1:B:62:ILE:HG13	1:B:106:VAL:HG13	1.79	0.65
1:C:34:PHE:CD2	1:C:36:ILE:HD11	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:LEU:O	1:D:49:LEU:HD23	1.98	0.64
1:D:14:GLU:HG2	1:D:308:CYS:SG	2.37	0.64
1:A:67:VAL:CG2	1:A:77:LEU:HD11	2.28	0.64
1:B:66:THR:HB	1:B:80:ARG:HD2	1.78	0.64
1:D:110:LEU:HD22	1:D:117:SER:OG	1.98	0.64
1:A:155:LEU:HD13	1:A:168:VAL:HG22	1.79	0.64
1:B:51:GLN:OE1	1:B:97:GLY:HA2	1.98	0.64
1:B:25:SER:O	1:B:29:ILE:HG12	1.97	0.63
1:C:40:ARG:NH2	1:C:45:LYS:O	2.31	0.63
1:B:290:VAL:HG13	1:B:325:PHE:CE2	2.33	0.63
1:C:133:ALA:HB3	1:C:155:LEU:HD21	1.80	0.63
1:C:203:ARG:O	1:C:203:ARG:HG2	1.97	0.63
1:B:60:THR:HG22	1:B:79:PHE:CE2	2.33	0.63
1:B:16:GLY:HA2	1:B:19:ILE:HG13	1.81	0.63
1:C:27:SER:O	1:C:81:PRO:HG3	1.99	0.63
1:A:324:ARG:NH2	1:D:76:ARG:NE	2.47	0.62
1:B:58:ALA:HA	1:B:91:PHE:CE1	2.34	0.62
1:B:60:THR:HG22	1:B:79:PHE:HE2	1.64	0.62
1:D:213:LEU:CD2	1:D:239:LEU:HD12	2.29	0.62
1:B:29:ILE:HD13	1:B:109:ALA:HA	1.81	0.62
1:C:300:GLU:HB3	1:C:337:SER:OG	2.00	0.62
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.65	0.62
1:C:137:ARG:NH1	1:C:155:LEU:H	1.97	0.62
1:C:131:PRO:HG3	1:C:284:TYR:OH	2.00	0.62
1:A:221:GLU:HG2	1:A:223:ASN:HD21	1.63	0.62
1:A:338:ILE:CG2	1:A:339:GLU:N	2.63	0.62
1:B:128:PRO:HD3	1:B:161:TYR:HB3	1.81	0.62
1:B:264:ALA:O	1:B:268:VAL:HG23	1.99	0.62
1:B:90:ARG:HG2	1:B:120:GLU:HB3	1.81	0.62
1:B:158:HIS:H	1:B:231:GLN:NE2	1.97	0.62
1:C:264:ALA:O	1:C:268:VAL:HG23	1.99	0.62
1:D:198:LEU:HD22	1:D:201:VAL:HB	1.81	0.62
1:B:79:PHE:CE1	1:B:81:PRO:HB3	2.34	0.62
1:C:13:GLY:HA3	1:C:312:THR:CG2	2.30	0.61
1:A:29:ILE:HD13	1:A:109:ALA:HA	1.82	0.61
1:A:58:ALA:HA	1:A:91:PHE:CE2	2.35	0.61
1:A:175:VAL:HG11	1:A:178:PHE:CE1	2.35	0.61
1:C:120:GLU:OE2	1:C:167:VAL:HG13	1.99	0.61
1:D:79:PHE:HE1	1:D:81:PRO:HB3	1.65	0.61
1:D:143:LEU:O	1:D:147:ILE:HG13	2.00	0.61
1:D:40:ARG:HD2	1:D:52:HIS:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HD21	1:C:227:LEU:CD1	2.31	0.61
1:A:125:THR:HG21	1:A:155:LEU:HD11	1.83	0.61
1:B:67:VAL:HG11	1:B:70:ALA:HB2	1.83	0.61
1:A:125:THR:CG2	1:A:155:LEU:HD11	2.30	0.61
1:A:254:GLY:HA2	1:A:263:VAL:HG21	1.83	0.61
1:C:30:THR:HG21	1:C:320:PHE:HD2	1.65	0.61
1:D:13:GLY:HA3	1:D:312:THR:HG21	1.81	0.60
1:D:175:VAL:HG11	1:D:178:PHE:CZ	2.35	0.60
1:D:298:ALA:C	1:D:338:ILE:HD12	2.25	0.60
1:B:293:MSE:HB3	1:B:338:ILE:CD1	2.31	0.60
1:B:5:MSE:HE1	1:B:78:LEU:CD1	2.32	0.60
1:D:156:LEU:HD13	1:D:167:VAL:HG12	1.82	0.60
1:B:130:ALA:HB1	1:B:131:PRO:HD2	1.83	0.60
1:C:201:VAL:HG12	1:C:205:VAL:HG21	1.83	0.60
1:D:293:MSE:HB3	1:D:338:ILE:CD1	2.19	0.60
1:C:58:ALA:HA	1:C:91:PHE:CE2	2.36	0.60
1:C:93:ILE:HD11	1:C:99:CYS:HA	1.82	0.60
1:D:135:PHE:CZ	1:D:140:LEU:HD13	2.36	0.60
1:B:68:GLU:HB2	1:B:78:LEU:HB3	1.82	0.60
1:B:330:THR:O	1:B:331:ASP:HB2	2.02	0.60
1:B:197:LEU:CD2	1:B:225:HIS:HB3	2.27	0.60
1:B:79:PHE:HE1	1:B:81:PRO:HB3	1.66	0.59
1:D:6:ILE:CD1	1:D:32:GLN:HE21	2.15	0.59
1:A:198:LEU:HD21	1:A:206:ALA:HB2	1.83	0.59
1:C:45:LYS:HA	1:C:45:LYS:HE2	1.83	0.59
1:A:16:GLY:CA	1:A:19:ILE:HG13	2.32	0.59
1:C:128:PRO:HA	1:C:253:VAL:HB	1.84	0.59
1:A:294:ALA:HA	1:A:338:ILE:CD1	2.33	0.59
1:D:28:MSE:HE2	1:D:59:ALA:HB1	1.84	0.59
1:D:30:THR:OG1	1:D:32:GLN:HG3	2.03	0.59
1:D:137:ARG:HA	1:D:141:GLU:OE1	2.02	0.59
1:D:197:LEU:HD23	1:D:225:HIS:HB3	1.85	0.59
1:D:33:PRO:HB3	1:D:80:ARG:HA	1.84	0.59
1:D:239:LEU:CD1	1:D:271:VAL:HG21	2.18	0.59
1:B:270:GLU:HA	1:B:273:ARG:HD3	1.84	0.59
1:C:16:GLY:CA	1:C:19:ILE:HD12	2.32	0.59
1:C:8:LEU:HD12	1:C:36:ILE:CD1	2.32	0.59
1:C:323:VAL:HG13	1:C:338:ILE:HG23	1.84	0.59
1:B:193:ARG:HH11	1:B:193:ARG:CG	2.15	0.58
1:B:160:PHE:CD2	1:B:234:GLY:HA3	2.38	0.58
1:C:68:GLU:HB2	1:C:78:LEU:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:THR:HG23	1:B:136:ILE:HD11	1.85	0.58
1:B:110:LEU:HD22	1:B:117:SER:OG	2.04	0.58
1:A:138:ARG:HD2	1:A:249:ARG:NH1	2.19	0.58
1:B:199:ALA:O	1:B:233:PRO:HA	2.04	0.58
1:C:128:PRO:HD3	1:C:161:TYR:HB3	1.86	0.58
1:A:26:LEU:CD2	1:A:316:VAL:HG12	2.33	0.58
1:D:127:ASN:OD1	1:D:161:TYR:HB2	2.04	0.58
1:A:26:LEU:HD21	1:A:317:VAL:HA	1.86	0.57
1:A:93:ILE:HD11	1:A:121:VAL:HG12	1.86	0.57
1:C:327:LEU:HD22	1:C:336:VAL:HG22	1.86	0.57
1:D:160:PHE:CD2	1:D:234:GLY:HA3	2.40	0.57
1:A:130:ALA:HB1	1:A:131:PRO:HD2	1.86	0.57
1:A:303:VAL:CG1	1:A:334:THR:HG22	2.35	0.57
1:B:6:ILE:CG2	1:B:8:LEU:HD21	2.34	0.57
1:B:5:MSE:HE2	1:B:33:PRO:CB	2.20	0.57
1:D:40:ARG:CD	1:D:52:HIS:HE1	2.16	0.57
1:C:266:GLN:O	1:C:270:GLU:HG3	2.04	0.57
1:A:89:TYR:HB3	1:A:91:PHE:CE1	2.40	0.56
1:B:85:ARG:O	1:B:89:TYR:OH	2.23	0.56
1:C:246:ILE:HG12	1:C:247:THR:N	2.21	0.56
1:A:58:ALA:O	1:A:62:ILE:HG12	2.05	0.56
1:A:298:ALA:HA	1:A:338:ILE:HG22	1.87	0.56
1:A:327:LEU:HD21	1:A:336:VAL:HG22	1.85	0.56
1:B:237:VAL:HG22	1:B:267:LEU:HD12	1.86	0.56
1:C:308:CYS:O	1:C:312:THR:HG23	2.06	0.56
1:C:112:PHE:N	1:C:112:PHE:CD1	2.72	0.56
1:D:217:PHE:CE2	1:D:268:VAL:HG22	2.39	0.56
1:A:29:ILE:HG23	1:A:112:PHE:HE2	1.70	0.56
1:C:45:LYS:HB3	1:C:49:LEU:HD21	1.86	0.56
1:A:298:ALA:HA	1:A:338:ILE:CG2	2.36	0.56
1:B:13:GLY:HA3	1:B:312:THR:HG22	1.87	0.56
1:C:34:PHE:HE1	1:C:79:PHE:CD2	2.24	0.56
1:A:128:PRO:HA	1:A:253:VAL:HB	1.86	0.56
1:A:189:ILE:HD11	1:A:275:LEU:HD11	1.88	0.56
1:B:18:GLN:CD	1:B:18:GLN:H	2.14	0.56
1:B:18:GLN:CD	1:B:18:GLN:N	2.64	0.56
1:C:249:ARG:HD3	1:C:251:PHE:CZ	2.40	0.56
1:C:40:ARG:HD3	1:C:52:HIS:CE1	2.34	0.55
1:C:62:ILE:HG13	1:C:106:VAL:HG13	1.89	0.55
1:D:45:LYS:HB2	1:D:49:LEU:HD11	1.88	0.55
1:B:290:VAL:HG12	1:B:317:VAL:HG21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:TRP:HB2	1:C:112:PHE:CD1	2.40	0.55
1:C:258:VAL:CG1	1:C:263:VAL:HG22	2.37	0.55
1:B:201:VAL:HG13	1:B:202:PRO:HD2	1.87	0.55
1:D:98:SER:HB3	1:D:101:LEU:CD1	2.35	0.55
1:A:230:ASP:C	1:A:232:GLY:H	2.13	0.55
1:B:199:ALA:HB2	1:B:227:LEU:HD12	1.88	0.55
1:A:18:GLN:HG2	1:A:309:HIS:NE2	2.22	0.55
1:A:158:HIS:HB2	1:A:231:GLN:HG2	1.89	0.55
1:A:329:GLU:HB3	1:B:327:LEU:H	1.72	0.55
1:C:175:VAL:HG11	1:C:178:PHE:CZ	2.41	0.55
1:C:5:MSE:HE2	1:C:33:PRO:HB2	1.89	0.55
1:B:40:ARG:NH2	1:B:49:LEU:HG	2.20	0.55
1:D:192:MSE:SE	1:D:217:PHE:CD1	3.10	0.55
1:A:46:PRO:HB2	1:A:75:GLN:NE2	2.20	0.55
1:C:284:TYR:O	1:C:288:GLN:HG2	2.07	0.55
1:A:140:LEU:O	1:A:141:GLU:C	2.50	0.54
1:B:58:ALA:O	1:B:62:ILE:HG12	2.06	0.54
1:B:66:THR:HB	1:B:80:ARG:HB2	1.89	0.54
1:D:52:HIS:O	1:D:56:VAL:HG23	2.07	0.54
1:B:68:GLU:CD	1:B:78:LEU:HD22	2.32	0.54
1:C:67:VAL:HG11	1:C:70:ALA:HB2	1.88	0.54
1:A:246:ILE:HG12	1:A:247:THR:N	2.23	0.54
1:B:13:GLY:HA3	1:B:312:THR:HG21	1.90	0.54
1:B:50:ARG:HG3	1:B:72:LEU:HD21	1.90	0.54
1:B:161:TYR:CD1	1:B:162:PRO:HA	2.42	0.54
1:A:197:LEU:O	1:A:235:ASN:HA	2.08	0.54
1:B:125:THR:OG1	1:B:159:GLY:N	2.37	0.54
1:D:48:LEU:C	1:D:49:LEU:HD23	2.33	0.54
1:D:141:GLU:HA	1:D:144:LEU:HD22	1.90	0.54
1:B:52:HIS:O	1:B:56:VAL:HG23	2.07	0.53
1:B:198:LEU:HD11	1:B:206:ALA:HB2	1.90	0.53
1:C:89:TYR:HB3	1:C:91:PHE:CE1	2.43	0.53
1:C:206:ALA:HB1	1:C:224:ILE:HG12	1.90	0.53
1:C:221:GLU:HB3	1:C:223:ASN:ND2	2.19	0.53
1:C:291:LEU:HD12	1:C:291:LEU:O	2.08	0.53
1:A:157:ARG:HD3	1:A:165:GLY:O	2.08	0.53
1:C:111:TRP:HB3	1:C:175:VAL:HG23	1.91	0.53
1:D:20:LEU:O	1:D:24:LEU:HD22	2.08	0.53
1:D:34:PHE:HE1	1:D:36:ILE:CG1	2.20	0.53
1:D:338:ILE:HG22	1:D:339:GLU:N	2.23	0.53
1:A:90:ARG:HH11	1:A:90:ARG:CG	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:VAL:HG12	1:A:334:THR:HG22	1.90	0.53
1:D:130:ALA:HB1	1:D:131:PRO:HD2	1.90	0.53
1:A:52:HIS:O	1:A:56:VAL:HG23	2.08	0.53
1:B:201:VAL:CG1	1:B:202:PRO:HD2	2.38	0.53
1:C:16:GLY:HA2	1:C:19:ILE:HD12	1.90	0.53
1:D:192:MSE:SE	1:D:217:PHE:HD1	2.42	0.53
1:D:230:ASP:C	1:D:232:GLY:H	2.16	0.53
1:C:111:TRP:HB2	1:C:112:PHE:HD1	1.73	0.53
1:A:208:ARG:NH1	1:A:208:ARG:HG2	2.24	0.53
1:B:33:PRO:HB3	1:B:80:ARG:HA	1.91	0.53
1:B:129:SER:O	1:B:130:ALA:HB2	2.09	0.53
1:A:44:ALA:HA	1:B:44:ALA:HA	1.91	0.53
1:D:5:MSE:HE1	1:D:78:LEU:HG	1.89	0.53
1:D:338:ILE:HG22	1:D:339:GLU:H	1.74	0.53
1:A:112:PHE:CZ	1:A:295:LEU:HD13	2.44	0.52
1:B:291:LEU:HB3	1:B:292:PRO:CD	2.36	0.52
1:C:39:ILE:HG22	1:C:40:ARG:HG3	1.91	0.52
1:B:29:ILE:HD12	1:B:112:PHE:CE2	2.44	0.52
1:C:34:PHE:HE2	1:C:36:ILE:HD11	1.69	0.52
1:D:20:LEU:HD22	1:D:24:LEU:CD2	2.38	0.52
1:D:136:ILE:HA	1:D:140:LEU:HD22	1.91	0.52
1:D:192:MSE:CE	1:D:275:LEU:HD21	2.29	0.52
1:C:192:MSE:HA	1:C:240:GLU:O	2.08	0.52
1:B:14:GLU:HA	1:B:14:GLU:OE1	2.08	0.52
1:C:107:LEU:HD13	1:C:170:THR:HG21	1.91	0.52
1:A:49:LEU:HD12	1:A:50:ARG:H	1.75	0.52
1:B:5:MSE:CE	1:B:78:LEU:HD11	2.38	0.52
1:A:46:PRO:O	1:A:75:GLN:NE2	2.42	0.52
1:B:26:LEU:HG	1:B:320:PHE:HB2	1.92	0.52
1:C:301:PHE:CD1	1:C:301:PHE:C	2.88	0.52
1:B:40:ARG:HH21	1:B:45:LYS:HB2	1.73	0.52
1:B:191:GLN:OE1	1:B:220:HIS:ND1	2.43	0.52
1:C:68:GLU:OE1	1:C:78:LEU:HD22	2.09	0.52
1:A:284:TYR:O	1:A:288:GLN:HG2	2.09	0.52
1:B:157:ARG:NH1	1:B:231:GLN:HA	2.24	0.52
1:C:314:ILE:HG23	1:C:325:PHE:CD1	2.44	0.52
1:A:129:SER:O	1:A:130:ALA:HB2	2.09	0.52
1:B:284:TYR:O	1:B:288:GLN:HG2	2.09	0.52
1:C:237:VAL:CG2	1:C:267:LEU:HD12	2.31	0.52
1:A:147:ILE:HG22	1:A:147:ILE:O	2.10	0.51
1:C:143:LEU:HD21	1:C:285:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:HG2	1:A:208:ARG:HH11	1.74	0.51
1:A:303:VAL:O	1:A:334:THR:HG22	2.10	0.51
1:C:237:VAL:HG11	1:C:263:VAL:HG12	1.91	0.51
1:B:40:ARG:HD2	1:B:43:ARG:HD2	1.92	0.51
1:C:67:VAL:HA	1:C:78:LEU:O	2.10	0.51
1:C:129:SER:O	1:C:130:ALA:HB2	2.10	0.51
1:D:12:GLN:O	1:D:19:ILE:HD11	2.10	0.51
1:B:18:GLN:HE21	1:B:21:ARG:HH12	1.56	0.51
1:A:40:ARG:NH2	1:A:45:LYS:HB2	2.25	0.51
1:A:93:ILE:HD11	1:A:121:VAL:HG11	1.93	0.51
1:B:197:LEU:O	1:B:235:ASN:HA	2.11	0.51
1:D:129:SER:O	1:D:130:ALA:HB2	2.11	0.51
1:B:60:THR:HG21	1:B:67:VAL:CG2	2.41	0.51
1:C:303:VAL:CG1	1:C:334:THR:HG22	2.41	0.51
1:D:34:PHE:CE1	1:D:36:ILE:HG12	2.43	0.51
1:D:83:THR:HB	1:D:85:ARG:HE	1.75	0.51
1:A:128:PRO:HD3	1:A:161:TYR:HB3	1.93	0.51
1:A:221:GLU:CG	1:A:223:ASN:HD21	2.23	0.51
1:B:136:ILE:HG23	1:B:140:LEU:HD21	1.92	0.51
1:C:60:THR:HG21	1:C:67:VAL:HG21	1.92	0.51
1:D:193:ARG:HB2	1:D:193:ARG:HH11	1.75	0.51
1:A:328:ILE:HG22	1:A:330:THR:HG23	1.91	0.51
1:B:93:ILE:HD11	1:B:99:CYS:HA	1.92	0.51
1:D:8:LEU:HD21	1:D:319:ARG:HG2	1.93	0.51
1:D:87:GLY:O	1:D:89:TYR:CD2	2.64	0.51
1:A:26:LEU:HD23	1:A:316:VAL:CG1	2.37	0.50
1:A:27:SER:O	1:A:81:PRO:HG3	2.11	0.50
1:B:16:GLY:CA	1:B:19:ILE:HG13	2.42	0.50
1:B:147:ILE:O	1:B:147:ILE:HG22	2.09	0.50
1:B:172:VAL:HG12	1:B:173:SER:H	1.77	0.50
1:C:293:MSE:O	1:C:338:ILE:HD12	2.11	0.50
1:C:338:ILE:HG22	1:C:339:GLU:N	2.26	0.50
1:D:26:LEU:C	1:D:30:THR:HG22	2.34	0.50
1:D:191:GLN:HG3	1:D:220:HIS:HB2	1.94	0.50
1:A:58:ALA:HA	1:A:91:PHE:HE2	1.76	0.50
1:B:293:MSE:HE1	1:B:301:PHE:CD2	2.47	0.50
1:C:237:VAL:HG22	1:C:267:LEU:CD1	2.29	0.50
1:C:193:ARG:NH1	1:C:240:GLU:OE2	2.44	0.50
1:A:254:GLY:HA2	1:A:263:VAL:CG2	2.42	0.50
1:D:137:ARG:HH11	1:D:155:LEU:HB2	1.76	0.50
1:D:192:MSE:HE1	1:D:275:LEU:CD2	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ILE:HG21	1:A:280:ALA:O	2.11	0.50
1:C:204:HIS:HA	1:C:207:GLU:HG2	1.93	0.49
1:C:5:MSE:HG3	1:C:33:PRO:HG2	1.93	0.49
1:D:60:THR:HG21	1:D:67:VAL:HG21	1.94	0.49
1:B:24:LEU:O	1:B:28:MSE:HG3	2.12	0.49
1:B:149:ILE:HA	1:B:175:VAL:HG22	1.95	0.49
1:D:314:ILE:HD13	1:D:325:PHE:CG	2.48	0.49
1:B:172:VAL:HG12	1:B:173:SER:N	2.28	0.49
1:C:217:PHE:HB2	1:C:219:LEU:HD21	1.94	0.49
1:A:258:VAL:HG12	1:A:263:VAL:HG23	1.94	0.49
1:B:5:MSE:HG2	1:B:33:PRO:HG2	1.95	0.49
1:A:90:ARG:HG2	1:A:90:ARG:NH1	2.08	0.49
1:A:189:ILE:HD11	1:A:275:LEU:CD1	2.43	0.49
1:C:8:LEU:CD2	1:C:319:ARG:HG2	2.43	0.49
1:C:136:ILE:HA	1:C:140:LEU:CD2	2.43	0.49
1:D:76:ARG:HG2	1:D:77:LEU:N	2.27	0.49
1:C:304:ALA:C	1:C:305:HIS:HD1	2.20	0.49
1:D:269:LYS:O	1:D:273:ARG:HG3	2.12	0.49
1:D:72:LEU:HD22	1:D:72:LEU:O	2.13	0.49
1:C:68:GLU:CD	1:C:78:LEU:HD22	2.37	0.49
1:D:69:GLY:O	1:D:71:GLU:N	2.42	0.49
1:C:230:ASP:C	1:C:232:GLY:N	2.70	0.48
1:D:186:ARG:NH2	1:D:277:SER:O	2.45	0.48
1:A:237:VAL:HG22	1:A:267:LEU:HD12	1.94	0.48
1:C:16:GLY:H	1:C:19:ILE:CD1	2.26	0.48
1:D:133:ALA:HB3	1:D:155:LEU:HD21	1.96	0.48
1:A:93:ILE:HD12	1:A:102:VAL:HG21	1.95	0.48
1:A:189:ILE:HD12	1:A:192:MSE:HE2	1.95	0.48
1:D:49:LEU:O	1:D:50:ARG:C	2.56	0.48
1:D:140:LEU:HD23	1:D:141:GLU:N	2.28	0.48
1:A:14:GLU:HA	1:B:14:GLU:OE1	2.14	0.48
1:C:140:LEU:O	1:C:141:GLU:C	2.56	0.48
1:A:67:VAL:HA	1:A:78:LEU:O	2.14	0.48
1:A:62:ILE:HG13	1:A:106:VAL:HG22	1.94	0.48
1:B:36:ILE:HB	1:B:39:ILE:CD1	2.43	0.48
1:C:111:TRP:CE2	1:C:149:ILE:HG21	2.49	0.48
1:C:201:VAL:CG1	1:C:205:VAL:HG21	2.44	0.48
1:D:252:VAL:HG21	1:D:266:GLN:HB2	1.95	0.48
1:A:148:GLY:O	1:A:150:HIS:CE1	2.66	0.48
1:B:110:LEU:HD22	1:B:117:SER:CB	2.44	0.48
1:A:29:ILE:HD12	1:A:112:PHE:HE2	1.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:LEU:O	1:B:24:LEU:HD22	2.13	0.48
1:C:298:ALA:HA	1:C:338:ILE:HB	1.96	0.48
1:D:128:PRO:HD2	1:D:161:TYR:HB3	1.95	0.48
1:D:284:TYR:O	1:D:287:ASP:HB2	2.14	0.48
1:A:20:LEU:O	1:A:24:LEU:HD13	2.14	0.48
1:B:154:THR:HG22	1:B:155:LEU:O	2.14	0.48
1:D:310:LEU:HD23	1:D:314:ILE:HG13	1.96	0.48
1:A:34:PHE:CE1	1:A:79:PHE:HB3	2.49	0.48
1:B:258:VAL:HG12	1:B:263:VAL:HG23	1.96	0.48
1:C:18:GLN:CD	1:C:18:GLN:H	2.22	0.48
1:C:246:ILE:HD13	1:C:280:ALA:O	2.13	0.48
1:C:318:GLU:HG2	1:C:323:VAL:O	2.14	0.48
1:D:48:LEU:HB3	1:D:53:LEU:HD13	1.96	0.48
1:C:8:LEU:HD21	1:C:319:ARG:HG2	1.96	0.47
1:D:12:GLN:HG2	1:D:19:ILE:HD13	1.95	0.47
1:D:20:LEU:HD22	1:D:24:LEU:HD21	1.96	0.47
1:A:26:LEU:HG	1:A:320:PHE:HB2	1.96	0.47
1:B:5:MSE:CE	1:B:33:PRO:HB2	2.22	0.47
1:B:155:LEU:HD22	1:B:168:VAL:HG22	1.95	0.47
1:C:303:VAL:HG12	1:C:334:THR:CG2	2.44	0.47
1:D:45:LYS:HA	1:D:46:PRO:HD2	1.41	0.47
1:B:111:TRP:O	1:B:174:PRO:HA	2.14	0.47
1:C:186:ARG:HG2	1:C:243:SER:CB	2.45	0.47
1:C:302:THR:HB	1:C:333:VAL:CG1	2.44	0.47
1:D:137:ARG:NH1	1:D:155:LEU:H	2.12	0.47
1:A:131:PRO:HG3	1:A:284:TYR:CZ	2.49	0.47
1:B:122:SER:HA	1:B:166:GLY:O	2.14	0.47
1:A:46:PRO:CB	1:A:75:GLN:HE21	2.27	0.47
1:D:193:ARG:HH11	1:D:193:ARG:CB	2.27	0.47
1:A:196:VAL:HG23	1:A:210:ILE:HD11	1.96	0.47
1:B:101:LEU:HD23	1:B:104:GLN:NE2	2.30	0.47
1:C:129:SER:O	1:C:130:ALA:CB	2.62	0.47
1:C:249:ARG:HD3	1:C:251:PHE:CE2	2.50	0.47
1:D:197:LEU:O	1:D:235:ASN:HA	2.14	0.47
1:D:284:TYR:CD1	1:D:284:TYR:C	2.92	0.47
1:A:128:PRO:HD3	1:A:161:TYR:CB	2.44	0.47
1:B:62:ILE:HD13	1:B:89:TYR:CE1	2.49	0.47
1:B:111:TRP:HZ3	1:B:295:LEU:CD1	2.28	0.47
1:C:34:PHE:CE1	1:C:79:PHE:CB	2.90	0.47
1:C:338:ILE:CG2	1:C:339:GLU:N	2.77	0.47
1:D:192:MSE:HA	1:D:240:GLU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:O	1:D:213:LEU:HB2	2.14	0.47
1:A:199:ALA:O	1:A:233:PRO:HA	2.14	0.47
1:C:111:TRP:C	1:C:112:PHE:CD1	2.93	0.47
1:D:121:VAL:HG12	1:D:122:SER:N	2.30	0.47
1:A:112:PHE:HZ	1:A:295:LEU:HD13	1.80	0.47
1:A:127:ASN:OD1	1:A:161:TYR:HB2	2.14	0.47
1:B:284:TYR:CE1	1:B:288:GLN:NE2	2.83	0.47
1:A:93:ILE:CD1	1:A:102:VAL:HG21	2.45	0.47
1:B:101:LEU:HD23	1:B:104:GLN:HE21	1.80	0.46
1:B:213:LEU:HD21	1:B:267:LEU:CD1	2.45	0.46
1:C:291:LEU:HD12	1:C:295:LEU:HG	1.97	0.46
1:A:266:GLN:O	1:A:269:LYS:HB2	2.15	0.46
1:C:227:LEU:HD13	1:C:231:GLN:HE21	1.80	0.46
1:D:9:ASP:O	1:D:12:GLN:HB3	2.15	0.46
1:A:167:VAL:HG12	1:A:167:VAL:O	2.16	0.46
1:C:301:PHE:CE1	1:C:336:VAL:HB	2.51	0.46
1:C:323:VAL:CG1	1:C:338:ILE:HG23	2.44	0.46
1:D:212:THR:HB	1:D:264:ALA:HB1	1.96	0.46
1:D:298:ALA:HA	1:D:338:ILE:HB	1.97	0.46
1:A:101:LEU:HA	1:A:104:GLN:HG2	1.98	0.46
1:A:300:GLU:HB3	1:A:337:SER:HA	1.96	0.46
1:A:317:VAL:HG13	1:A:321:LEU:HD12	1.97	0.46
1:B:87:GLY:O	1:B:89:TYR:CD2	2.68	0.46
1:B:111:TRP:HB3	1:B:175:VAL:HG23	1.97	0.46
1:B:136:ILE:HA	1:B:140:LEU:CD2	2.44	0.46
1:B:188:ASN:O	1:B:244:GLU:HG3	2.15	0.46
1:C:204:HIS:HA	1:C:207:GLU:CG	2.46	0.46
1:D:172:VAL:CG1	1:D:173:SER:H	2.21	0.46
1:D:241:VAL:HG11	1:D:274:TYR:HE2	1.81	0.46
1:A:195:GLU:HA	1:A:223:ASN:O	2.16	0.46
1:C:6:ILE:HG23	1:C:319:ARG:NH1	2.31	0.46
1:C:58:ALA:HA	1:C:91:PHE:HE2	1.79	0.46
1:C:199:ALA:O	1:C:233:PRO:HA	2.15	0.46
1:C:330:THR:O	1:C:331:ASP:HB2	2.14	0.46
1:A:140:LEU:HD23	1:A:141:GLU:N	2.30	0.46
1:A:338:ILE:HG23	1:A:339:GLU:H	1.81	0.46
1:C:196:VAL:HG11	1:C:206:ALA:HA	1.97	0.46
1:A:45:LYS:HA	1:A:45:LYS:CE	2.43	0.46
1:A:48:LEU:HD12	1:A:74:SER:HB3	1.98	0.46
1:B:76:ARG:HG2	1:B:77:LEU:N	2.31	0.46
1:B:293:MSE:HE1	1:B:301:PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:CYS:O	1:C:64:GLY:C	2.59	0.46
1:B:38:SER:O	1:B:39:ILE:C	2.57	0.46
1:C:40:ARG:HH22	1:C:49:LEU:HD11	1.76	0.46
1:C:112:PHE:N	1:C:112:PHE:HD1	2.13	0.46
1:D:140:LEU:O	1:D:141:GLU:C	2.59	0.46
1:A:238:SER:HA	1:A:267:LEU:HD11	1.97	0.45
1:B:66:THR:CB	1:B:80:ARG:HD2	2.45	0.45
1:C:229:ARG:O	1:C:232:GLY:N	2.50	0.45
1:D:328:ILE:HG22	1:D:330:THR:HG23	1.98	0.45
1:A:45:LYS:HA	1:A:46:PRO:HD2	1.52	0.45
1:C:303:VAL:HG12	1:C:334:THR:HG22	1.98	0.45
1:D:38:SER:O	1:D:39:ILE:C	2.58	0.45
1:A:66:THR:HB	1:A:80:ARG:HB2	1.99	0.45
1:A:181:LEU:CD2	1:A:183:LEU:HD21	2.47	0.45
1:A:249:ARG:HD3	1:A:251:PHE:CZ	2.52	0.45
1:C:259:SER:HB3	1:C:262:VAL:HG23	1.98	0.45
1:C:289:LEU:O	1:C:292:PRO:HG2	2.15	0.45
1:B:29:ILE:CD1	1:B:109:ALA:HA	2.47	0.45
1:D:50:ARG:HG3	1:D:50:ARG:HH11	1.82	0.45
1:B:129:SER:O	1:B:130:ALA:CB	2.64	0.45
1:B:149:ILE:CG1	1:B:178:PHE:HE1	2.30	0.45
1:B:267:LEU:HD22	1:B:271:VAL:HG23	1.99	0.45
1:D:47:GLY:HA3	1:D:74:SER:O	2.16	0.45
1:D:327:LEU:CD2	1:D:336:VAL:HG22	2.43	0.45
1:B:198:LEU:HB2	1:B:226:ASN:OD1	2.17	0.45
1:B:279:ALA:HA	1:B:302:THR:OG1	2.17	0.45
1:C:48:LEU:HB3	1:C:53:LEU:HD12	1.99	0.45
1:C:71:GLU:O	1:C:73:GLY:N	2.48	0.45
1:A:125:THR:HG23	1:A:133:ALA:HB3	1.99	0.45
1:A:141:GLU:OE2	1:A:153:THR:N	2.49	0.45
1:A:153:THR:HG23	1:A:170:THR:OG1	2.17	0.45
1:B:93:ILE:HG13	1:B:122:SER:O	2.17	0.45
1:B:189:ILE:CG2	1:B:190:VAL:N	2.79	0.45
1:A:51:GLN:HG2	1:A:97:GLY:HA2	1.99	0.45
1:C:38:SER:O	1:C:39:ILE:C	2.59	0.45
1:D:132:PRO:O	1:D:135:PHE:HB3	2.17	0.45
1:C:39:ILE:HB	1:C:75:GLN:HA	1.99	0.45
1:C:185:GLU:O	1:C:245:ASN:ND2	2.49	0.45
1:A:102:VAL:O	1:A:105:THR:HB	2.17	0.44
1:A:246:ILE:HG12	1:A:247:THR:H	1.82	0.44
1:B:92:ALA:HA	1:B:122:SER:OG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ILE:HG22	1:B:330:THR:CG2	2.45	0.44
1:C:48:LEU:HB3	1:C:53:LEU:CD1	2.47	0.44
1:C:60:THR:HB	1:C:65:ALA:HB3	1.97	0.44
1:C:237:VAL:CG1	1:C:263:VAL:HG12	2.47	0.44
1:D:39:ILE:HG13	1:D:75:GLN:O	2.17	0.44
1:A:46:PRO:C	1:A:75:GLN:HE21	2.25	0.44
1:A:129:SER:O	1:A:130:ALA:CB	2.64	0.44
1:B:28:MSE:HE2	1:B:59:ALA:HB1	1.99	0.44
1:C:189:ILE:HA	1:C:243:SER:HA	1.98	0.44
1:D:246:ILE:CG1	1:D:247:THR:N	2.80	0.44
1:B:198:LEU:HD22	1:B:201:VAL:HB	1.98	0.44
1:D:93:ILE:CG1	1:D:122:SER:O	2.66	0.44
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.76	0.44
1:A:111:TRP:HB3	1:A:175:VAL:HG23	1.98	0.44
1:B:189:ILE:HD13	1:B:192:MSE:HE3	2.00	0.44
1:B:196:VAL:HG11	1:B:206:ALA:CA	2.46	0.44
1:B:230:ASP:C	1:B:232:GLY:H	2.25	0.44
1:A:22:SER:HB2	1:A:316:VAL:HG11	1.99	0.44
1:B:139:VAL:CG2	1:B:249:ARG:HB3	2.48	0.44
1:C:210:ILE:HG22	1:C:211:ALA:N	2.30	0.44
1:A:36:ILE:O	1:A:36:ILE:HG22	2.18	0.44
1:A:138:ARG:CD	1:A:249:ARG:NH1	2.80	0.44
1:B:271:VAL:HG12	1:B:275:LEU:HD22	1.98	0.44
1:C:175:VAL:HG11	1:C:178:PHE:CE2	2.53	0.44
1:D:128:PRO:CD	1:D:161:TYR:HB3	2.48	0.44
1:D:271:VAL:HG12	1:D:275:LEU:CD2	2.45	0.44
1:A:316:VAL:O	1:A:317:VAL:C	2.61	0.44
1:B:26:LEU:HD13	1:B:26:LEU:HA	1.57	0.44
1:C:108:PRO:HA	1:C:111:TRP:CD2	2.52	0.44
1:D:259:SER:HB2	1:D:262:VAL:HG23	1.98	0.44
1:C:289:LEU:O	1:C:290:VAL:C	2.59	0.44
1:A:108:PRO:HA	1:A:111:TRP:CD2	2.52	0.44
1:B:20:LEU:HD22	1:B:24:LEU:HD22	1.99	0.44
1:B:22:SER:OG	1:B:316:VAL:HG11	2.18	0.44
1:B:52:HIS:N	1:B:52:HIS:CD2	2.86	0.44
1:B:157:ARG:CD	1:B:165:GLY:O	2.65	0.44
1:C:36:ILE:HD12	1:C:36:ILE:HG23	1.69	0.44
1:C:39:ILE:HD11	1:C:77:LEU:HB2	2.00	0.44
1:D:129:SER:O	1:D:130:ALA:CB	2.65	0.44
1:D:157:ARG:HD2	1:D:165:GLY:O	2.17	0.44
1:D:258:VAL:HG13	1:D:262:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ARG:HH11	1:A:208:ARG:CG	2.31	0.43
1:A:318:GLU:HG2	1:A:323:VAL:O	2.19	0.43
1:B:16:GLY:H	1:B:19:ILE:CD1	2.28	0.43
1:B:20:LEU:HD22	1:B:24:LEU:CD2	2.48	0.43
1:B:197:LEU:HD23	1:B:225:HIS:CB	2.36	0.43
1:C:133:ALA:CB	1:C:155:LEU:HD21	2.45	0.43
1:C:192:MSE:C	1:C:193:ARG:HG3	2.43	0.43
1:D:93:ILE:HD13	1:D:102:VAL:HG21	2.00	0.43
1:D:246:ILE:HG12	1:D:247:THR:N	2.34	0.43
1:D:249:ARG:HD3	1:D:251:PHE:CZ	2.52	0.43
1:A:5:MSE:HG2	1:A:6:ILE:N	2.32	0.43
1:A:160:PHE:O	1:A:161:TYR:C	2.61	0.43
1:B:45:LYS:HB3	1:B:49:LEU:HD21	2.00	0.43
1:A:67:VAL:HG22	1:A:77:LEU:HD11	1.99	0.43
1:B:27:SER:HB2	1:B:34:PHE:CD2	2.52	0.43
1:C:5:MSE:HE1	1:C:78:LEU:CD1	2.44	0.43
1:C:297:GLY:O	1:C:298:ALA:HB2	2.18	0.43
1:A:40:ARG:HB3	1:A:43:ARG:HB2	2.00	0.43
1:A:186:ARG:HD3	1:A:274:TYR:CE2	2.53	0.43
1:A:324:ARG:NH2	1:D:76:ARG:HE	2.13	0.43
1:B:14:GLU:H	1:B:312:THR:HG21	1.83	0.43
1:B:21:ARG:CB	1:B:105:THR:HG23	2.45	0.43
1:B:192:MSE:HA	1:B:240:GLU:O	2.18	0.43
1:D:313:ASN:O	1:D:317:VAL:HG23	2.18	0.43
1:A:192:MSE:HA	1:A:240:GLU:O	2.19	0.43
1:D:107:LEU:HA	1:D:107:LEU:HD23	1.79	0.43
1:B:160:PHE:CG	1:B:234:GLY:HA3	2.54	0.43
1:C:33:PRO:HB3	1:C:80:ARG:HA	2.01	0.43
1:C:110:LEU:HD22	1:C:117:SER:OG	2.19	0.43
1:D:20:LEU:HD22	1:D:24:LEU:HD22	2.01	0.43
1:D:45:LYS:HA	1:D:45:LYS:CE	2.47	0.43
1:A:90:ARG:CG	1:A:90:ARG:NH1	2.76	0.43
1:A:90:ARG:HH12	1:A:118:ARG:NH2	2.17	0.43
1:B:338:ILE:HG22	1:B:339:GLU:N	2.32	0.43
1:C:14:GLU:H	1:C:312:THR:HG21	1.83	0.43
1:A:118:ARG:HG3	1:A:171:GLU:CD	2.44	0.43
1:A:303:VAL:HG12	1:A:334:THR:CG2	2.49	0.43
1:B:157:ARG:HD3	1:B:165:GLY:O	2.19	0.43
1:D:318:GLU:HG2	1:D:323:VAL:O	2.19	0.43
1:A:72:LEU:HD22	1:A:72:LEU:O	2.19	0.43
1:B:196:VAL:HG11	1:B:206:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:LEU:HD21	1:D:267:LEU:HD13	2.00	0.43
1:D:306:PRO:O	1:D:306:PRO:HG2	2.19	0.43
1:A:107:LEU:CD2	1:A:170:THR:HG21	2.48	0.42
1:D:6:ILE:O	1:D:34:PHE:HA	2.19	0.42
1:B:22:SER:O	1:B:26:LEU:HB2	2.19	0.42
1:C:34:PHE:CD2	1:C:36:ILE:CD1	3.02	0.42
1:C:223:ASN:ND2	1:C:223:ASN:N	2.65	0.42
1:C:301:PHE:C	1:C:301:PHE:HD1	2.26	0.42
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.85	0.42
1:B:62:ILE:HG13	1:B:106:VAL:CG1	2.47	0.42
1:B:290:VAL:HG13	1:B:325:PHE:CZ	2.54	0.42
1:D:125:THR:HG22	1:D:168:VAL:CG2	2.49	0.42
1:A:18:GLN:N	1:A:18:GLN:OE1	2.52	0.42
1:A:324:ARG:O	1:A:339:GLU:N	2.52	0.42
1:C:29:ILE:HG21	1:C:295:LEU:HD21	2.02	0.42
1:C:190:VAL:HB	1:C:242:GLU:HG2	2.01	0.42
1:C:228:PRO:HB2	1:C:230:ASP:HB2	2.01	0.42
1:C:49:LEU:O	1:C:50:ARG:C	2.62	0.42
1:C:88:ASP:OD1	1:C:118:ARG:HD3	2.19	0.42
1:C:255:GLU:HB2	1:C:258:VAL:CB	2.41	0.42
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.82	0.42
1:B:39:ILE:HG22	1:B:40:ARG:HG3	2.00	0.42
1:C:195:GLU:HG2	1:C:196:VAL:N	2.35	0.42
1:A:111:TRP:O	1:A:174:PRO:HA	2.20	0.42
1:A:230:ASP:C	1:A:232:GLY:N	2.78	0.42
1:B:99:CYS:O	1:B:100:THR:C	2.62	0.42
1:B:157:ARG:HH12	1:B:231:GLN:HA	1.84	0.42
1:C:26:LEU:O	1:C:30:THR:HG22	2.19	0.42
1:D:151:GLN:HG3	1:D:170:THR:HG21	2.02	0.42
1:A:6:ILE:O	1:A:34:PHE:HA	2.19	0.42
1:A:266:GLN:HA	1:A:269:LYS:HD2	2.02	0.42
1:B:189:ILE:HG22	1:B:190:VAL:N	2.35	0.42
1:C:202:PRO:C	1:C:204:HIS:H	2.28	0.42
1:C:325:PHE:HA	1:C:337:SER:O	2.20	0.42
1:D:38:SER:HA	1:D:75:GLN:HG2	2.02	0.42
1:D:39:ILE:HG21	1:D:48:LEU:CD2	2.50	0.42
1:D:310:LEU:O	1:D:314:ILE:HG13	2.20	0.42
1:A:107:LEU:HD13	1:A:151:GLN:OE1	2.20	0.41
1:A:303:VAL:HG13	1:A:334:THR:HG22	2.01	0.41
1:B:267:LEU:HD22	1:B:271:VAL:CG2	2.50	0.41
1:C:57:LYS:O	1:C:61:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:THR:HG22	1:C:106:VAL:N	2.35	0.41
1:D:18:GLN:CD	1:D:18:GLN:N	2.78	0.41
1:D:125:THR:HG21	1:D:155:LEU:HD11	2.01	0.41
1:A:190:VAL:O	1:A:191:GLN:HB3	2.21	0.41
1:B:40:ARG:O	1:B:41:ALA:C	2.62	0.41
1:C:246:ILE:CG1	1:C:247:THR:N	2.83	0.41
1:D:205:VAL:HG12	1:D:235:ASN:HD21	1.85	0.41
1:A:186:ARG:HG2	1:A:243:SER:CB	2.51	0.41
1:B:7:ALA:O	1:B:8:LEU:HD23	2.19	0.41
1:C:283:GLU:H	1:C:283:GLU:HG2	1.68	0.41
1:A:35:THR:HA	1:A:77:LEU:O	2.20	0.41
1:A:259:SER:O	1:A:260:ALA:C	2.63	0.41
1:B:67:VAL:HA	1:B:78:LEU:O	2.21	0.41
1:C:131:PRO:HA	1:C:132:PRO:HD3	1.61	0.41
1:C:182:GLN:HE21	1:C:182:GLN:HB2	1.70	0.41
1:D:111:TRP:HB2	1:D:112:PHE:CD1	2.56	0.41
1:D:141:GLU:N	1:D:142:PRO:CD	2.82	0.41
1:A:267:LEU:O	1:A:267:LEU:HD23	2.20	0.41
1:B:127:ASN:OD1	1:B:161:TYR:HB2	2.20	0.41
1:B:131:PRO:HA	1:B:132:PRO:HD3	1.93	0.41
1:B:141:GLU:HG2	1:B:151:GLN:O	2.21	0.41
1:B:196:VAL:HG23	1:B:210:ILE:HD11	2.02	0.41
1:C:45:LYS:HA	1:C:46:PRO:HD2	1.60	0.41
1:C:199:ALA:HB2	1:C:227:LEU:HB2	2.03	0.41
1:C:319:ARG:HG3	1:C:319:ARG:HH11	1.85	0.41
1:D:186:ARG:NH2	1:D:275:LEU:O	2.54	0.41
1:A:103:LEU:HG	1:A:121:VAL:HG21	2.02	0.41
1:A:125:THR:HG21	1:A:155:LEU:CD1	2.49	0.41
1:A:198:LEU:HD11	1:A:206:ALA:HB2	2.02	0.41
1:C:195:GLU:HA	1:C:223:ASN:O	2.21	0.41
1:D:160:PHE:O	1:D:161:TYR:C	2.61	0.41
1:A:237:VAL:HG11	1:A:263:VAL:HG12	2.03	0.41
1:C:290:VAL:HG12	1:C:291:LEU:N	2.35	0.41
1:D:141:GLU:HA	1:D:144:LEU:CD2	2.50	0.41
1:A:147:ILE:HD13	1:A:147:ILE:HG21	1.76	0.41
1:A:217:PHE:CE2	1:A:268:VAL:HG13	2.55	0.41
1:B:209:GLU:CD	1:B:235:ASN:HD21	2.29	0.41
1:C:29:ILE:HD11	1:C:108:PRO:O	2.20	0.41
1:C:327:LEU:HD23	1:C:336:VAL:HG22	2.02	0.41
1:A:38:SER:O	1:A:39:ILE:C	2.64	0.41
1:A:181:LEU:HD21	1:A:183:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:HB1	1:A:224:ILE:HG12	2.02	0.41
1:B:112:PHE:CE2	1:B:295:LEU:HD13	2.55	0.41
1:B:154:THR:HG22	1:B:155:LEU:N	2.36	0.41
1:B:191:GLN:HG3	1:B:193:ARG:HD2	2.02	0.41
1:B:242:GLU:HA	1:B:247:THR:HG23	2.02	0.41
1:B:258:VAL:HG12	1:B:263:VAL:CG2	2.51	0.41
1:B:324:ARG:O	1:B:339:GLU:N	2.53	0.41
1:C:5:MSE:CG	1:C:33:PRO:HG2	2.51	0.41
1:C:88:ASP:CG	1:C:118:ARG:HD3	2.46	0.41
1:D:13:GLY:HA3	1:D:312:THR:HG23	2.00	0.41
1:A:144:LEU:O	1:A:145:ALA:C	2.61	0.41
1:A:184:GLY:O	1:A:302:THR:OG1	2.39	0.41
1:A:217:PHE:CD2	1:A:239:LEU:HD11	2.56	0.41
1:A:325:PHE:HA	1:A:337:SER:O	2.20	0.41
1:C:153:THR:HG23	1:C:170:THR:OG1	2.21	0.41
1:C:227:LEU:HD13	1:C:231:GLN:NE2	2.35	0.41
1:D:321:LEU:HB3	1:D:322:PRO:HD2	2.03	0.41
1:A:29:ILE:CD1	1:A:112:PHE:CD2	2.97	0.40
1:A:196:VAL:HG23	1:A:210:ILE:CD1	2.51	0.40
1:C:53:LEU:O	1:C:57:LYS:HG3	2.21	0.40
1:C:238:SER:HA	1:C:267:LEU:HD11	2.04	0.40
1:D:48:LEU:HD11	1:D:77:LEU:CD1	2.44	0.40
1:A:281:VAL:O	1:A:303:VAL:HG23	2.21	0.40
1:A:93:ILE:HG12	1:A:93:ILE:H	1.64	0.40
1:A:99:CYS:O	1:A:100:THR:C	2.64	0.40
1:A:303:VAL:CG1	1:A:334:THR:CG2	2.99	0.40
1:B:135:PHE:CD2	1:B:284:TYR:HE2	2.40	0.40
1:C:72:LEU:HD22	1:C:72:LEU:O	2.21	0.40
1:C:266:GLN:O	1:C:269:LYS:HB2	2.22	0.40
1:D:22:SER:O	1:D:26:LEU:HD23	2.22	0.40
1:C:39:ILE:HD13	1:C:48:LEU:HD21	2.02	0.40
1:C:147:ILE:HG22	1:C:147:ILE:O	2.21	0.40
1:C:155:LEU:HD13	1:C:155:LEU:HA	1.37	0.40
1:C:303:VAL:CG1	1:C:334:THR:CG2	2.99	0.40
1:C:249:ARG:HG2	1:C:251:PHE:CZ	2.56	0.40
1:C:249:ARG:HH11	1:C:249:ARG:HD2	1.61	0.40
1:D:258:VAL:CG1	1:D:263:VAL:HG23	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/347 (96%)	291 (87%)	34 (10%)	8 (2%)	4	17
1	B	333/347 (96%)	295 (89%)	30 (9%)	8 (2%)	4	17
1	C	333/347 (96%)	293 (88%)	32 (10%)	8 (2%)	4	17
1	D	333/347 (96%)	294 (88%)	29 (9%)	10 (3%)	3	12
All	All	1332/1388 (96%)	1173 (88%)	125 (9%)	34 (3%)	4	15

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ILE
1	A	130	ALA
1	B	39	ILE
1	B	130	ALA
1	C	39	ILE
1	C	72	LEU
1	C	130	ALA
1	D	39	ILE
1	D	130	ALA
1	A	72	LEU
1	B	41	ALA
1	B	72	LEU
1	D	70	ALA
1	D	72	LEU
1	A	16	GLY
1	B	70	ALA
1	C	203	ARG
1	D	231	GLN
1	A	203	ARG
1	B	191	GLN
1	B	203	ARG
1	C	94	GLY

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Mol	Chain	Res	Type
1	D	41	ALA
1	D	203	ARG
1	C	46	PRO
1	C	184	GLY
1	D	94	GLY
1	D	276	ALA
1	A	46	PRO
1	B	184	GLY
1	A	94	GLY
1	D	184	GLY
1	A	184	GLY
1	C	16	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	262/269 (97%)	207 (79%)	55 (21%)	1	4
1	B	262/269 (97%)	214 (82%)	48 (18%)	2	6
1	C	262/269 (97%)	205 (78%)	57 (22%)	1	3
1	D	262/269 (97%)	212 (81%)	50 (19%)	1	5
All	All	1048/1076 (97%)	838 (80%)	210 (20%)	1	4

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	MSE
1	A	14	GLU
1	A	19	ILE
1	A	20	LEU
1	A	22	SER
1	A	26	LEU
1	A	30	THR
1	A	33	PRO
1	A	35	THR

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Mol	Chain	Res	Type
1	A	36	ILE
1	A	39	ILE
1	A	60	THR
1	A	72	LEU
1	A	90	ARG
1	A	93	ILE
1	A	95	SER
1	A	102	VAL
1	A	106	VAL
1	A	117	SER
1	A	120	GLU
1	A	121	VAL
1	A	140	LEU
1	A	141	GLU
1	A	142	PRO
1	A	143	LEU
1	A	144	LEU
1	A	149	ILE
1	A	154	THR
1	A	162	PRO
1	A	167	VAL
1	A	172	VAL
1	A	181	LEU
1	A	182	GLN
1	A	189	ILE
1	A	190	VAL
1	A	203	ARG
1	A	208	ARG
1	A	216	SER
1	A	220	HIS
1	A	231	GLN
1	A	237	VAL
1	A	238	SER
1	A	243	SER
1	A	248	GLU
1	A	261	GLU
1	A	272	LYS
1	A	275	LEU
1	A	300	GLU
1	A	309	HIS
1	A	310	LEU
1	A	312	THR

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Mol	Chain	Res	Type
1	A	326	SER
1	A	329	GLU
1	A	334	THR
1	A	338	ILE
1	B	5	MSE
1	B	14	GLU
1	B	19	ILE
1	B	20	LEU
1	B	24	LEU
1	B	26	LEU
1	B	37	THR
1	B	38	SER
1	B	39	ILE
1	B	49	LEU
1	B	53	LEU
1	B	72	LEU
1	B	78	LEU
1	B	90	ARG
1	B	93	ILE
1	B	105	THR
1	B	117	SER
1	B	125	THR
1	B	129	SER
1	B	140	LEU
1	B	141	GLU
1	B	142	PRO
1	B	143	LEU
1	B	144	LEU
1	B	152	GLN
1	B	155	LEU
1	B	162	PRO
1	B	181	LEU
1	B	192	MSE
1	B	193	ARG
1	B	216	SER
1	B	218	SER
1	B	222	GLN
1	B	225	HIS
1	B	231	GLN
1	B	237	VAL
1	B	248	GLU
1	B	255	GLU

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Mol	Chain	Res	Type
1	B	259	SER
1	B	267	LEU
1	B	270	GLU
1	B	275	LEU
1	B	277	SER
1	B	278	THR
1	B	281	VAL
1	B	291	LEU
1	B	303	VAL
1	B	310	LEU
1	C	5	MSE
1	C	14	GLU
1	C	20	LEU
1	C	26	LEU
1	C	27	SER
1	C	30	THR
1	C	35	THR
1	C	61	GLU
1	C	68	GLU
1	C	72	LEU
1	C	74	SER
1	C	93	ILE
1	C	100	THR
1	C	105	THR
1	C	108	PRO
1	C	112	PHE
1	C	117	SER
1	C	118	ARG
1	C	136	ILE
1	C	140	LEU
1	C	141	GLU
1	C	143	LEU
1	C	144	LEU
1	C	155	LEU
1	C	157	ARG
1	C	162	PRO
1	C	170	THR
1	C	171	GLU
1	C	172	VAL
1	C	173	SER
1	C	181	LEU
1	C	182	GLN

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Mol	Chain	Res	Type
1	C	197	LEU
1	C	205	VAL
1	C	210	ILE
1	C	212	THR
1	C	220	HIS
1	C	223	ASN
1	C	224	ILE
1	C	231	GLN
1	C	237	VAL
1	C	243	SER
1	C	244	GLU
1	C	248	GLU
1	C	258	VAL
1	C	267	LEU
1	C	277	SER
1	C	278	THR
1	C	283	GLU
1	C	291	LEU
1	C	310	LEU
1	C	316	VAL
1	C	317	VAL
1	C	329	GLU
1	C	335	ARG
1	C	337	SER
1	C	338	ILE
1	D	5	MSE
1	D	12	GLN
1	D	20	LEU
1	D	24	LEU
1	D	26	LEU
1	D	32	GLN
1	D	35	THR
1	D	36	ILE
1	D	51	GLN
1	D	53	LEU
1	D	66	THR
1	D	72	LEU
1	D	90	ARG
1	D	93	ILE
1	D	100	THR
1	D	102	VAL
1	D	108	PRO

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Mol	Chain	Res	Type
1	D	117	SER
1	D	120	GLU
1	D	128	PRO
1	D	132	PRO
1	D	140	LEU
1	D	141	GLU
1	D	144	LEU
1	D	147	ILE
1	D	155	LEU
1	D	157	ARG
1	D	162	PRO
1	D	181	LEU
1	D	188	ASN
1	D	189	ILE
1	D	193	ARG
1	D	216	SER
1	D	225	HIS
1	D	231	GLN
1	D	243	SER
1	D	248	GLU
1	D	255	GLU
1	D	261	GLU
1	D	267	LEU
1	D	268	VAL
1	D	275	LEU
1	D	278	THR
1	D	281	VAL
1	D	300	GLU
1	D	305	HIS
1	D	312	THR
1	D	314	ILE
1	D	323	VAL
1	D	333	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	151	GLN
1	A	182	GLN
1	A	223	ASN
1	A	225	HIS

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Mol	Chain	Res	Type
1	A	305	HIS
1	B	18	GLN
1	B	52	HIS
1	B	231	GLN
1	B	235	ASN
1	B	288	GLN
1	C	52	HIS
1	C	75	GLN
1	C	182	GLN
1	C	191	GLN
1	C	223	ASN
1	C	225	HIS
1	C	226	ASN
1	C	231	GLN
1	D	32	GLN
1	D	52	HIS
1	D	179	ASN
1	D	220	HIS
1	D	235	ASN
1	D	266	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 ⓘ

There are no ligands in this entry.

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

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	331/347 (95%)	-0.01	15 (4%) 38 30	2, 26, 97, 160	0
1	B	331/347 (95%)	0.05	15 (4%) 38 30	2, 29, 92, 186	0
1	C	331/347 (95%)	-0.02	13 (3%) 43 34	2, 27, 94, 141	0
1	D	331/347 (95%)	0.03	18 (5%) 31 24	2, 30, 99, 162	0
All	All	1324/1388 (95%)	0.01	61 (4%) 37 29	2, 28, 97, 186	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	HIS	5.1
1	B	232	GLY	4.8
1	B	46	PRO	4.2
1	C	96	ALA	3.7
1	D	37	THR	3.7
1	C	129	SER	3.4
1	A	330	THR	3.2
1	C	171	GLU	3.2
1	B	257	ARG	3.1
1	A	96	ALA	3.1
1	A	260	ALA	3.0
1	D	74	SER	3.0
1	A	259	SER	3.0
1	C	16	GLY	3.0
1	D	287	ASP	2.9
1	A	127	ASN	2.8
1	B	18	GLN	2.8
1	A	16	GLY	2.8
1	C	88	ASP	2.7
1	C	43	ARG	2.7
1	D	204	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	42	GLY	2.7
1	C	257	ARG	2.7
1	C	18	GLN	2.7
1	D	137	ARG	2.6
1	D	85	ARG	2.6
1	D	94	GLY	2.6
1	B	308	CYS	2.6
1	D	60	THR	2.5
1	A	339	GLU	2.5
1	D	257	ARG	2.4
1	D	220	HIS	2.4
1	D	283	GLU	2.4
1	C	131	PRO	2.4
1	A	74	SER	2.3
1	D	96	ALA	2.3
1	A	262	VAL	2.3
1	B	60	THR	2.3
1	D	46	PRO	2.3
1	D	244	GLU	2.3
1	A	332	GLY	2.3
1	B	31	GLY	2.3
1	B	171	GLU	2.2
1	C	266	GLN	2.2
1	C	150	HIS	2.2
1	B	45	LYS	2.2
1	D	40	ARG	2.1
1	B	204	HIS	2.1
1	A	45	LYS	2.1
1	A	41	ALA	2.1
1	D	45	LYS	2.1
1	D	331	ASP	2.1
1	B	43	ARG	2.1
1	C	229	ARG	2.1
1	A	185	GLU	2.1
1	B	339	GLU	2.1
1	C	256	LYS	2.0
1	A	257	ARG	2.0
1	B	64	GLY	2.0
1	D	57	LYS	2.0
1	A	37	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.