



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:44 AM UTC

PDB ID : 2A9G / pdb_00002a9g
Title : Structure of C406A arginine deiminase in complex with L-arginine
Authors : Galkin, A.; Lu, X.; Dunaway-Mariano, D.; Herzberg, O.
Deposited on : 2005-07-11
Resolution : 2.30 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

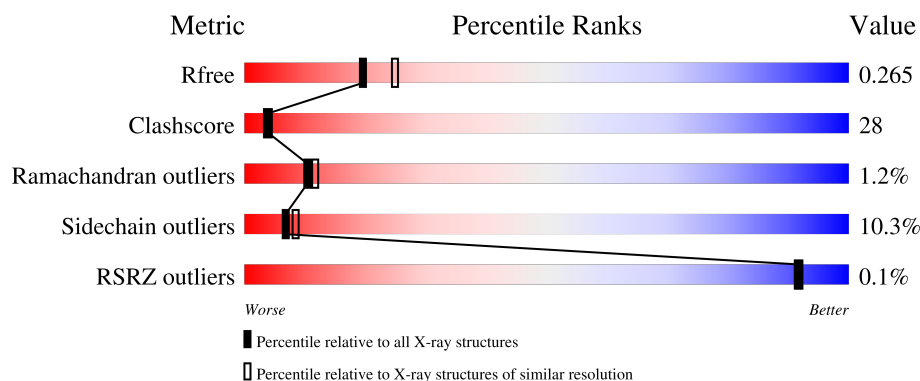
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	418	 45% 41% 10% . .
1	B	418	 54% 35% 7% . .
1	C	418	 54% 33% 9% .
1	D	418	 47% 40% 10% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13747 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.

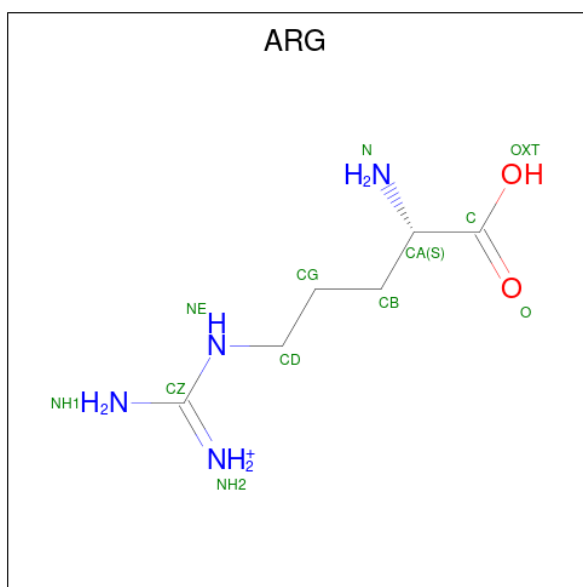
- Molecule 1 is a protein called Arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3163	2001	552	594	16			
1	B	405	Total	C	N	O	S	0	0	0
			3164	2002	552	594	16			
1	C	402	Total	C	N	O	S	0	0	0
			3141	1989	546	590	16			
1	D	406	Total	C	N	O	S	0	0	0
			3167	2003	553	595	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	406	ALA	CYS	engineered mutation	UNP P13981
B	406	ALA	CYS	engineered mutation	UNP P13981
C	406	ALA	CYS	engineered mutation	UNP P13981
D	406	ALA	CYS	engineered mutation	UNP P13981

- Molecule 2 is ARGININE (CCD ID: ARG) (formula: C₆H₁₅N₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	6	4	2		
2	B	1	Total	C	N	O	0	0
			12	6	4	2		
2	C	1	Total	C	N	O	0	0
			12	6	4	2		
2	D	1	Total	C	N	O	0	0
			12	6	4	2		

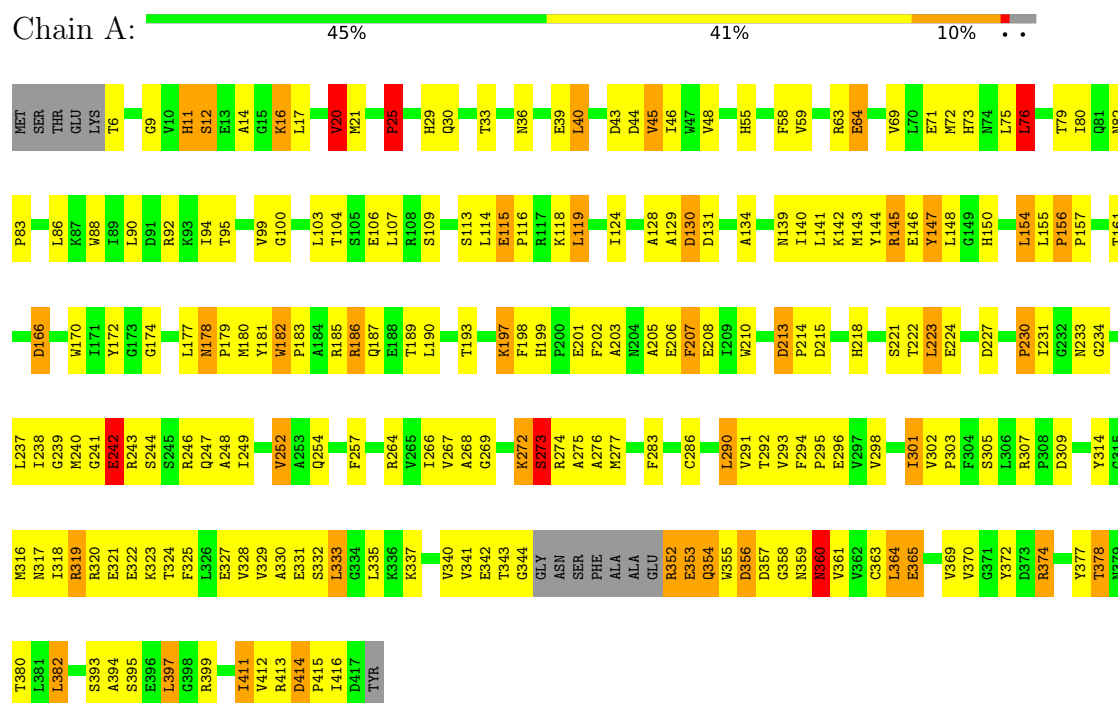
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	223	Total	O	0	0
			223	223		
3	B	277	Total	O	0	0
			277	277		
3	C	309	Total	O	0	0
			309	309		
3	D	255	Total	O	0	0
			255	255		

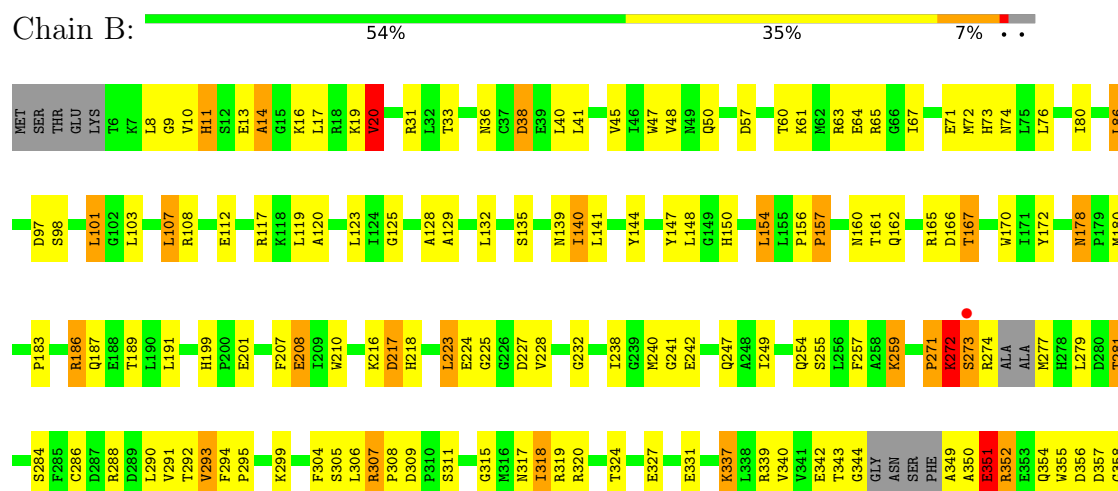
3 Residue-property plots

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

• Molecule 1: Arginine deiminase



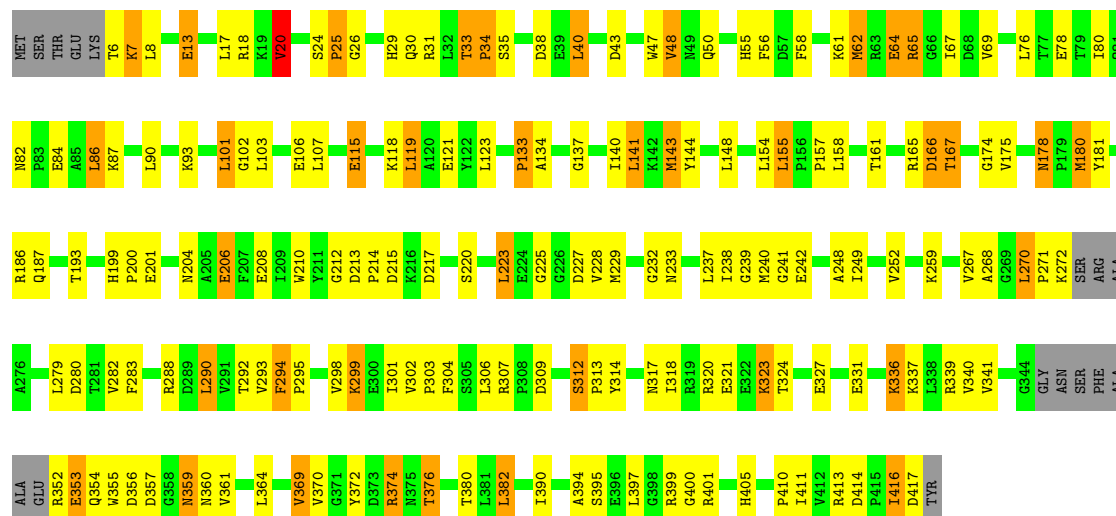
• Molecule 1: Arginine deiminase





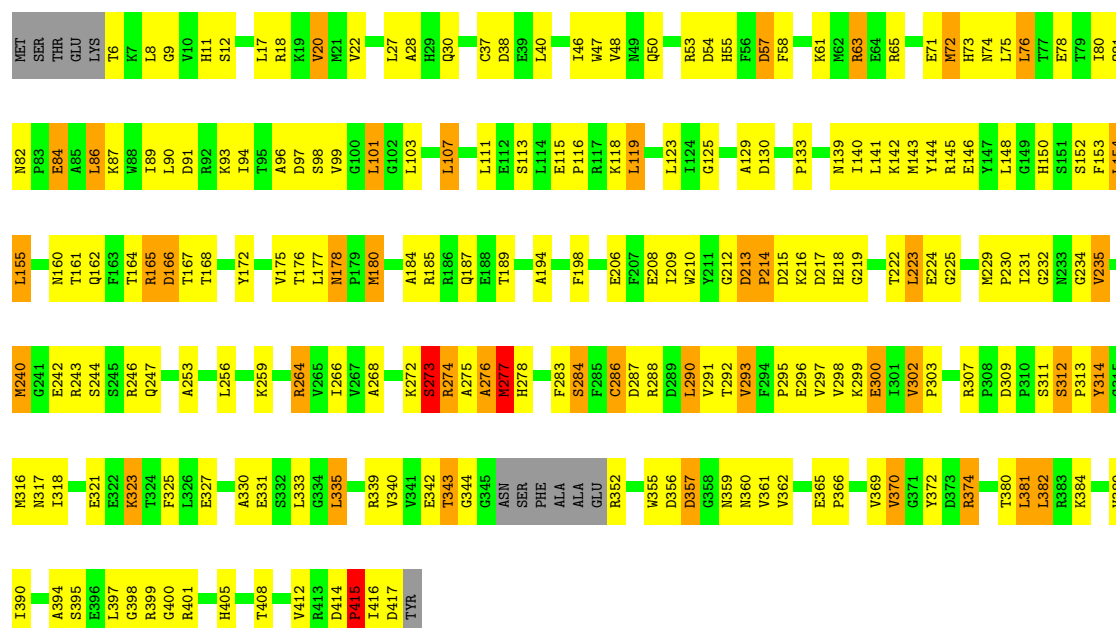
• Molecule 1: Arginine deiminase

Chain C: 54% 33% 9%



• Molecule 1: Arginine deiminase

Chain D: 47% 40% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.10Å 120.70Å 151.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 99.0 (20.00-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.267 0.199 , 0.265	Depositor DCC
R_{free} test set	2001 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13747	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.78	0/3230	1.30	42/4381 (1.0%)
1	B	0.86	3/3230 (0.1%)	1.36	43/4379 (1.0%)
1	C	0.84	1/3207 (0.0%)	1.28	33/4349 (0.8%)
1	D	0.82	2/3234 (0.1%)	1.26	31/4386 (0.7%)
All	All	0.82	6/12901 (0.0%)	1.30	149/17495 (0.9%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13	GLU	N-CA	6.14	1.53	1.46
1	D	297	VAL	N-CA	5.66	1.52	1.45
1	C	13	GLU	N-CA	5.50	1.53	1.46
1	D	370	VAL	CA-CB	-5.35	1.47	1.54
1	B	366	PRO	N-CA	5.09	1.53	1.47
1	B	318	ILE	CA-CB	5.05	1.61	1.54

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	273	SER	N-CA-C	17.42	131.79	110.19
1	C	48	VAL	N-CA-C	10.55	120.54	110.42
1	A	234	GLY	N-CA-C	-10.51	100.61	115.43
1	C	178	ASN	N-CA-C	9.91	122.14	109.65
1	B	354	GLN	OE1-CD-NE2	-9.71	112.89	122.60
1	A	178	ASN	N-CA-C	9.45	121.65	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	LEU	N-CA-C	-8.82	101.61	111.14
1	B	272	LYS	CA-C-N	8.62	136.29	121.29
1	B	272	LYS	C-N-CA	8.62	136.29	121.29
1	A	161	THR	N-CA-C	-8.46	102.22	112.54
1	B	294	PHE	CA-C-N	8.39	130.33	119.84
1	B	294	PHE	C-N-CA	8.39	130.33	119.84
1	A	340	VAL	N-CA-C	8.32	120.77	108.45
1	C	166	ASP	N-CA-C	8.28	121.50	111.40
1	A	364	LEU	N-CA-C	-8.21	103.21	113.55
1	B	359	ASN	N-CA-C	-8.10	100.09	110.53
1	B	154	LEU	N-CA-C	-7.94	101.72	111.40
1	C	312	SER	N-CA-C	7.79	119.72	109.83
1	C	340	VAL	N-CA-C	7.68	118.86	108.11
1	C	115	GLU	N-CA-C	-7.66	100.00	109.65
1	B	361	VAL	N-CA-C	-7.58	101.79	110.05
1	C	181	TYR	N-CA-C	7.42	119.16	111.14
1	B	48	VAL	N-CA-C	7.40	118.13	110.36
1	A	361	VAL	N-CA-C	-7.37	102.02	110.05
1	B	272	LYS	N-CA-C	7.36	120.36	110.35
1	B	11	HIS	CA-CB-CG	-7.31	106.49	113.80
1	B	16	LYS	N-CA-C	7.30	119.66	109.15
1	A	354	GLN	N-CA-C	7.29	119.38	110.41
1	B	144	TYR	N-CA-C	-7.28	103.35	111.28
1	C	161	THR	N-CA-C	-7.16	103.48	111.71
1	A	64	GLU	N-CA-C	-7.08	103.12	114.09
1	A	20	VAL	CB-CA-C	-7.07	99.38	110.69
1	B	178	ASN	N-CA-C	7.07	119.89	109.50
1	A	166	ASP	N-CA-C	7.02	121.93	113.23
1	C	282	VAL	N-CA-C	-6.99	106.49	113.20
1	B	354	GLN	CG-CD-NE2	6.93	126.80	116.40
1	B	161	THR	N-CA-C	-6.89	103.79	111.71
1	B	140	ILE	N-CA-C	-6.84	103.67	110.30
1	D	214	PRO	CA-N-CD	-6.82	102.46	112.00
1	D	166	ASP	N-CA-C	6.79	118.47	111.14
1	D	161	THR	N-CA-C	-6.74	104.16	112.38
1	D	286	CYS	N-CA-C	-6.71	105.72	114.04
1	B	273	SER	CA-C-N	6.69	133.75	121.70
1	B	273	SER	C-N-CA	6.69	133.75	121.70
1	D	374	ARG	N-CA-C	6.68	119.40	111.71
1	D	57	ASP	N-CA-C	-6.64	104.12	111.36
1	D	189	THR	N-CA-C	6.61	118.49	111.28
1	A	114	LEU	N-CA-C	6.57	119.28	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	PRO	CA-C-N	6.56	127.54	120.13
1	A	156	PRO	C-N-CA	6.56	127.54	120.13
1	B	228	VAL	N-CA-C	6.52	117.69	108.36
1	A	45	VAL	N-CA-C	-6.48	102.89	110.21
1	A	48	VAL	N-CA-C	6.44	117.12	110.36
1	C	13	GLU	N-CA-C	6.43	121.29	113.38
1	D	178	ASN	N-CA-C	6.39	118.89	109.50
1	A	30	GLN	N-CA-C	-6.37	104.77	112.54
1	A	294	PHE	CA-C-N	6.37	127.80	119.84
1	A	294	PHE	C-N-CA	6.37	127.80	119.84
1	D	276	ALA	CB-CA-C	-6.31	109.31	116.63
1	D	415	PRO	CA-N-CD	-6.25	103.25	112.00
1	D	48	VAL	N-CA-C	6.17	116.92	110.62
1	D	154	LEU	N-CA-C	-6.07	104.29	111.03
1	A	182	TRP	CA-C-N	-6.07	112.61	119.28
1	A	182	TRP	C-N-CA	-6.07	112.61	119.28
1	A	25	PRO	CA-C-N	-6.05	117.50	122.16
1	A	25	PRO	C-N-CA	-6.05	117.50	122.16
1	A	365	GLU	N-CA-C	-6.04	101.25	108.25
1	C	13	GLU	N-CA-CB	-6.02	101.55	110.53
1	B	340	VAL	N-CA-C	5.94	117.04	108.48
1	B	166	ASP	N-CA-C	5.94	120.71	112.45
1	D	96	ALA	N-CA-C	-5.91	105.92	113.01
1	B	11	HIS	CB-CA-C	-5.81	101.67	111.02
1	C	312	SER	CA-C-N	5.80	125.47	119.56
1	C	312	SER	C-N-CA	5.80	125.47	119.56
1	A	203	ALA	N-CA-C	5.79	120.92	111.37
1	C	359	ASN	N-CA-C	-5.75	103.12	110.53
1	D	155	LEU	N-CA-C	-5.73	101.67	110.32
1	D	297	VAL	N-CA-C	5.72	118.69	112.96
1	D	37	CYS	N-CA-C	5.72	118.29	111.71
1	B	186	ARG	N-CA-C	5.72	118.25	111.33
1	A	393	SER	N-CA-C	5.70	117.96	109.59
1	A	273	SER	CA-C-N	-5.69	111.50	120.60
1	A	273	SER	C-N-CA	-5.69	111.50	120.60
1	A	11	HIS	N-CA-C	5.68	119.52	112.59
1	C	123	LEU	N-CA-C	-5.67	105.09	111.28
1	B	156	PRO	N-CA-C	5.67	117.61	110.70
1	A	414	ASP	CA-C-N	5.67	126.92	119.84
1	A	414	ASP	C-N-CA	5.67	126.92	119.84
1	C	292	THR	N-CA-C	-5.65	101.08	110.17
1	C	212	GLY	N-CA-C	5.65	118.62	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	LEU	N-CA-C	5.62	118.70	109.72
1	B	398	GLY	N-CA-C	5.59	120.61	114.40
1	B	364	LEU	N-CA-C	-5.59	106.59	113.41
1	D	300	GLU	N-CA-CB	-5.58	101.77	110.98
1	A	198	PHE	N-CA-C	5.58	121.11	113.97
1	C	40	LEU	N-CA-C	-5.57	106.08	112.92
1	C	121	GLU	N-CA-C	-5.57	105.21	111.28
1	B	20	VAL	CB-CA-C	-5.56	101.79	110.69
1	B	191	LEU	N-CA-C	5.54	117.32	111.28
1	D	72	MET	N-CA-C	5.54	117.76	111.11
1	C	309	ASP	CA-C-N	5.52	125.35	119.28
1	C	309	ASP	C-N-CA	5.52	125.35	119.28
1	A	230	PRO	N-CA-C	-5.52	101.10	112.47
1	B	366	PRO	CB-CA-C	5.52	118.65	111.64
1	B	389	VAL	N-CA-C	5.51	114.68	106.85
1	C	374	ARG	N-CA-C	5.51	118.22	111.82
1	B	189	THR	N-CA-C	5.50	116.95	111.07
1	D	153	PHE	N-CA-C	5.49	117.05	109.15
1	D	335	LEU	N-CA-C	5.47	118.16	109.24
1	B	16	LYS	O-C-N	5.46	130.14	122.77
1	A	186	ARG	N-CA-C	5.46	117.99	111.71
1	D	414	ASP	N-CA-C	5.45	118.05	110.20
1	D	339	ARG	N-CA-C	-5.44	101.42	110.17
1	C	270	LEU	CA-C-N	5.43	125.42	120.21
1	C	270	LEU	C-N-CA	5.43	125.42	120.21
1	B	376	THR	N-CA-C	5.42	117.19	111.28
1	A	119	LEU	N-CA-C	-5.40	105.30	111.07
1	C	294	PHE	CA-C-N	5.36	126.54	119.84
1	C	294	PHE	C-N-CA	5.36	126.54	119.84
1	D	414	ASP	O-C-N	5.35	127.27	121.60
1	A	213	ASP	CA-C-N	5.34	126.52	119.84
1	A	213	ASP	C-N-CA	5.34	126.52	119.84
1	D	382	LEU	N-CA-C	-5.32	105.48	111.28
1	D	94	ILE	N-CA-C	5.32	114.40	106.85
1	C	314	TYR	N-CA-C	-5.31	106.03	112.88
1	A	76	LEU	N-CA-C	-5.30	105.20	110.97
1	C	376	THR	N-CA-C	5.27	117.03	111.28
1	C	7	LYS	N-CA-C	5.27	117.67	110.55
1	D	284	SER	N-CA-C	5.27	117.97	108.48
1	D	302	VAL	CA-C-N	5.27	125.72	120.14
1	D	302	VAL	C-N-CA	5.27	125.72	120.14
1	C	217	ASP	N-CA-C	-5.25	100.61	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	PRO	N-CA-C	-5.25	103.20	111.34
1	B	157	PRO	N-CA-C	-5.24	103.05	111.38
1	B	241	GLY	N-CA-C	5.24	121.06	114.25
1	B	390	ILE	N-CA-C	-5.22	102.00	108.89
1	B	210	TRP	N-CA-C	5.21	117.63	111.33
1	A	411	ILE	N-CA-C	-5.20	107.75	112.12
1	A	252	VAL	CB-CA-C	-5.18	105.30	112.24
1	A	374	ARG	N-CA-C	5.17	119.34	113.19
1	C	20	VAL	N-CA-C	5.13	116.04	108.45
1	B	292	THR	N-CA-C	-5.12	102.17	110.32
1	B	339	ARG	N-CA-C	-5.11	102.72	110.28
1	C	137	GLY	N-CA-C	-5.11	106.58	112.50
1	D	240	MET	N-CA-C	5.09	117.54	109.50
1	D	209	ILE	CB-CA-C	-5.09	106.14	112.45
1	B	232	GLY	N-CA-C	-5.08	106.47	111.85
1	B	14	ALA	N-CA-C	5.07	119.54	112.90
1	C	228	VAL	N-CA-C	5.05	116.23	108.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	TYR	Sidechain

5.2 Too-close contacts [i](#)

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	3163	0	3151	209	0
1	B	3164	0	3152	155	0
1	C	3141	0	3127	169	0
1	D	3167	0	3154	194	0
2	A	12	0	12	0	0
2	B	12	0	12	2	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
3	A	223	0	0	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	277	0	0	32	0
3	C	309	0	0	46	0
3	D	255	0	0	46	0
All	All	13747	0	12632	703	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 28.

All (703) 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:14:ALA:O	1:B:366:PRO:HD3	1.34	1.22
1:D:276:ALA:HA	3:D:4622:HOH:O	1.42	1.19
1:B:242:GLU:OE2	1:B:273:SER:HB3	1.42	1.19
1:A:247:GLN:HG2	3:D:4733:HOH:O	1.42	1.16
1:B:73:HIS:HB3	1:B:117:ARG:HH12	1.04	1.14
1:A:317:ASN:HB2	3:A:1699:HOH:O	1.47	1.13
1:C:410:PRO:HD2	3:C:3796:HOH:O	1.48	1.09
1:C:331:GLU:HB2	3:C:3771:HOH:O	1.55	1.07
1:C:33:THR:HG22	1:C:35:SER:H	1.22	1.04
1:D:416:ILE:HG23	1:D:417:ASP:H	1.22	1.04
1:B:101:LEU:HD12	1:B:101:LEU:H	1.19	1.02
1:A:40:LEU:HD11	3:A:1709:HOH:O	1.62	0.98
1:C:199:HIS:HD2	1:C:201:GLU:H	1.10	0.98
1:D:293:VAL:HG22	1:D:298:VAL:HG21	1.44	0.97
1:C:240:MET:HE3	1:C:267:VAL:HG11	1.43	0.97
1:C:354:GLN:HE22	1:D:47:TRP:HA	1.31	0.95
1:A:267:VAL:HG13	3:A:1703:HOH:O	1.66	0.95
1:D:63:ARG:HG2	3:D:4730:HOH:O	1.65	0.94
1:D:357:ASP:HB2	3:D:4613:HOH:O	1.68	0.94
1:B:304:PHE:HB3	1:B:318:ILE:HD11	1.50	0.93
1:B:8:LEU:HB2	3:B:2760:HOH:O	1.69	0.93
1:B:207:PHE:HB3	3:B:2760:HOH:O	1.66	0.93
1:D:76:LEU:O	1:D:80:ILE:HG12	1.69	0.91
1:A:80:ILE:HB	1:A:86:LEU:HD13	1.51	0.91
1:A:104:THR:HG22	3:A:1721:HOH:O	1.71	0.90
1:B:73:HIS:HB3	1:B:117:ARG:NH1	1.85	0.90
1:D:103:LEU:HD13	1:D:154:LEU:HD11	1.54	0.90
1:D:323:LYS:HG2	1:D:327:GLU:HB3	1.53	0.90
1:C:416:ILE:HG22	1:C:417:ASP:OD1	1.71	0.90
1:A:395:SER:OG	1:B:395:SER:HB3	1.71	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:CYS:HB2	1:A:290:LEU:HD13	1.54	0.89
1:B:242:GLU:OE2	1:B:273:SER:CB	2.22	0.87
1:D:231:ILE:HD13	1:D:333:LEU:HD21	1.56	0.86
1:B:286:CYS:HB2	1:B:290:LEU:HD12	1.58	0.86
1:B:101:LEU:H	1:B:101:LEU:CD1	1.90	0.85
1:D:231:ILE:HD13	1:D:333:LEU:CD2	2.07	0.85
1:C:208:GLU:HG2	1:C:210:TRP:CZ3	2.12	0.84
1:D:333:LEU:HB2	1:D:335:LEU:HD12	1.57	0.84
1:B:349:ALA:HA	3:B:2749:HOH:O	1.78	0.84
1:B:304:PHE:HE1	1:C:143:MET:HE3	1.43	0.83
1:D:416:ILE:HA	3:D:4739:HOH:O	1.77	0.83
1:D:97:ASP:C	3:D:4733:HOH:O	2.22	0.83
1:C:33:THR:HG22	1:C:35:SER:N	1.93	0.83
1:A:33:THR:HG22	1:A:36:ASN:CG	2.04	0.82
1:D:65:ARG:HH11	1:D:65:ARG:HG3	1.43	0.82
1:A:83:PRO:HA	3:A:1563:HOH:O	1.78	0.82
1:D:17:LEU:HD21	1:D:20:VAL:CG1	2.09	0.82
1:B:374:ARG:HD2	3:B:2538:HOH:O	1.80	0.82
1:D:142:LYS:HA	3:D:4751:HOH:O	1.79	0.82
1:C:199:HIS:CD2	1:C:201:GLU:H	1.97	0.82
1:C:323:LYS:HB3	1:C:327:GLU:OE1	1.80	0.81
1:A:344:GLY:HA3	3:A:1689:HOH:O	1.79	0.81
1:D:416:ILE:HG23	1:D:417:ASP:N	1.96	0.81
1:A:134:ALA:HA	3:A:1648:HOH:O	1.81	0.81
1:B:165:ARG:HD3	1:B:405:HIS:O	1.81	0.80
1:D:76:LEU:HD22	1:D:80:ILE:HD11	1.64	0.80
1:A:148:LEU:HD13	3:A:1717:HOH:O	1.82	0.79
1:C:240:MET:HG2	1:C:241:GLY:N	1.97	0.79
1:C:240:MET:HE3	1:C:267:VAL:CG1	2.12	0.79
1:D:234:GLY:HA2	3:D:4578:HOH:O	1.81	0.79
1:D:17:LEU:HD21	1:D:20:VAL:HG11	1.64	0.77
1:D:180:MET:HE3	1:D:224:GLU:HG2	1.67	0.77
1:D:38:ASP:HB3	3:D:4743:HOH:O	1.85	0.77
1:D:111:LEU:O	1:D:119:LEU:HD22	1.85	0.77
1:A:63:ARG:C	3:A:1504:HOH:O	2.28	0.77
1:C:270:LEU:HD21	3:C:3786:HOH:O	1.84	0.76
1:A:238:ILE:HG21	1:A:249:ILE:HG12	1.68	0.76
1:C:279:LEU:HA	3:C:3786:HOH:O	1.86	0.76
1:A:72:MET:HE3	3:A:1615:HOH:O	1.85	0.75
1:B:17:LEU:HD11	1:B:20:VAL:HG13	1.67	0.75
1:D:288:ARG:HD2	3:D:4600:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ALA:O	1:A:252:VAL:HG23	1.87	0.74
1:D:357:ASP:N	1:D:357:ASP:OD1	2.20	0.74
1:C:240:MET:CE	1:C:267:VAL:HG11	2.18	0.74
1:A:318:ILE:HD12	1:D:140:ILE:HD13	1.68	0.73
1:B:361:VAL:HB	1:B:369:VAL:HG13	1.70	0.73
1:A:103:LEU:HD13	1:A:154:LEU:HD11	1.70	0.73
1:C:376:THR:O	1:C:380:THR:HG23	1.88	0.73
1:A:140:ILE:HD12	1:A:144:TYR:CE2	2.23	0.73
1:A:186:ARG:NH1	3:A:1645:HOH:O	2.21	0.73
1:A:377:TYR:CE2	3:A:1531:HOH:O	2.42	0.73
1:B:342:GLU:O	1:B:352:ARG:NH2	2.22	0.73
1:D:145:ARG:HD2	3:D:4644:HOH:O	1.87	0.73
1:C:31:ARG:HD2	1:C:157:PRO:HB3	1.71	0.72
1:A:240:MET:HB2	3:A:1703:HOH:O	1.89	0.72
1:B:255:SER:O	1:B:259:LYS:HD3	1.89	0.72
1:D:129:ALA:HB2	1:D:141:LEU:HD12	1.71	0.72
1:B:60:THR:HA	3:B:2772:HOH:O	1.90	0.72
1:B:352:ARG:NE	3:B:2667:HOH:O	2.21	0.72
1:A:298:VAL:O	1:A:301:ILE:HG22	1.90	0.72
1:A:178:ASN:HB3	1:A:223:LEU:O	1.89	0.72
1:A:303:PRO:HG2	1:A:321:GLU:HB2	1.71	0.72
1:B:363:CYS:O	1:B:413:ARG:NH2	2.23	0.72
1:A:183:PRO:HA	1:A:186:ARG:HD2	1.73	0.71
1:C:103:LEU:HD22	1:C:154:LEU:HD11	1.72	0.71
1:B:119:LEU:HD23	1:B:119:LEU:O	1.90	0.71
1:B:286:CYS:HB2	1:B:290:LEU:CD1	2.20	0.71
1:C:180:MET:HA	1:C:180:MET:HE2	1.71	0.71
1:A:156:PRO:HG3	1:A:187:GLN:NE2	2.05	0.70
1:A:143:MET:O	1:A:147:TYR:HB2	1.91	0.70
1:A:372:TYR:CG	1:A:394:ALA:HB2	2.27	0.70
1:C:214:PRO:HD2	3:C:3697:HOH:O	1.91	0.70
1:C:293:VAL:HG13	1:C:298:VAL:HG21	1.74	0.70
1:A:72:MET:CE	3:A:1615:HOH:O	2.38	0.70
1:C:87:LYS:HE2	3:C:3804:HOH:O	1.92	0.70
1:C:101:LEU:HG	3:C:3775:HOH:O	1.91	0.70
1:B:216:LYS:HE2	3:B:2651:HOH:O	1.91	0.70
1:B:352:ARG:CZ	3:B:2667:HOH:O	2.40	0.70
1:C:232:GLY:O	1:C:233:ASN:HB2	1.92	0.69
1:D:416:ILE:CG2	1:D:417:ASP:H	2.02	0.69
1:C:206:GLU:HG2	3:C:3688:HOH:O	1.91	0.69
1:D:216:LYS:HD3	1:D:218:HIS:CE1	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:LYS:HG3	1:D:327:GLU:OE1	1.93	0.69
1:D:416:ILE:HG13	3:D:4739:HOH:O	1.90	0.69
1:A:140:ILE:HD12	1:A:144:TYR:CZ	2.28	0.69
1:B:295:PRO:O	1:B:299:LYS:HG2	1.93	0.69
1:D:107:LEU:HD22	1:D:111:LEU:CD1	2.23	0.69
1:D:229:MET:HE1	1:D:283:PHE:CD2	2.28	0.69
1:A:364:LEU:HD11	1:A:370:VAL:CG2	2.23	0.69
1:A:178:ASN:HB2	1:A:180:MET:CE	2.23	0.68
1:B:401:ARG:NH2	3:B:2736:HOH:O	2.24	0.68
1:B:208:GLU:OE1	1:B:208:GLU:HA	1.92	0.68
1:C:18:ARG:NH1	1:C:414:ASP:OD2	2.27	0.68
1:D:361:VAL:HG22	3:D:4725:HOH:O	1.91	0.68
1:D:111:LEU:HD22	1:D:119:LEU:HD13	1.76	0.68
1:A:363:CYS:O	1:A:413:ARG:NH2	2.27	0.68
1:C:175:VAL:HG12	3:C:3784:HOH:O	1.93	0.68
1:D:318:ILE:HG23	1:D:318:ILE:O	1.94	0.68
1:C:178:ASN:HB3	1:C:223:LEU:O	1.94	0.68
1:D:229:MET:HE1	1:D:283:PHE:HD2	1.59	0.68
1:B:288:ARG:HG3	1:B:288:ARG:HH11	1.59	0.67
1:C:140:ILE:HA	1:C:143:MET:HE2	1.76	0.67
1:B:14:ALA:O	1:B:366:PRO:CD	2.27	0.67
1:D:99:VAL:HG13	1:D:154:LEU:HD12	1.76	0.67
1:D:370:VAL:HG22	1:D:390:ILE:HB	1.75	0.67
1:D:57:ASP:OD1	1:D:61:LYS:HE3	1.95	0.67
1:D:98:SER:N	3:D:4733:HOH:O	2.26	0.67
1:A:150:HIS:NE2	3:A:1717:HOH:O	2.27	0.67
1:D:288:ARG:HB3	1:D:416:ILE:HD11	1.77	0.67
1:D:103:LEU:CD1	1:D:154:LEU:HD11	2.25	0.67
1:A:94:ILE:CG2	3:A:1721:HOH:O	2.42	0.67
1:D:256:LEU:HD12	3:D:4747:HOH:O	1.94	0.66
1:A:25:PRO:HA	1:A:29:HIS:CE1	2.31	0.66
1:D:65:ARG:HH11	1:D:65:ARG:CG	2.08	0.66
1:C:13:GLU:HG3	1:C:229:MET:HE2	1.77	0.66
1:C:17:LEU:HD21	1:C:20:VAL:HG11	1.77	0.66
1:D:12:SER:HB2	3:D:4599:HOH:O	1.94	0.66
1:A:94:ILE:HG22	3:A:1721:HOH:O	1.96	0.66
1:A:240:MET:HE2	1:A:246:ARG:HA	1.78	0.66
1:C:355:TRP:CH2	1:C:357:ASP:HB2	2.31	0.66
1:C:405:HIS:HE1	3:C:3781:HOH:O	1.78	0.66
1:A:174:GLY:HA3	1:A:210:TRP:CE2	2.32	0.65
1:D:235:VAL:HG13	1:D:264:ARG:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:354:GLN:NE2	1:D:47:TRP:HA	2.06	0.65
1:C:341:VAL:HG21	1:C:382:LEU:HD12	1.78	0.65
1:B:293:VAL:O	1:B:295:PRO:HD3	1.97	0.65
1:C:242:GLU:OE2	1:C:272:LYS:HG2	1.97	0.65
1:A:182:TRP:HB3	3:A:1515:HOH:O	1.96	0.65
1:B:307:ARG:HD2	3:B:2582:HOH:O	1.96	0.64
1:A:80:ILE:HD11	1:A:116:PRO:HA	1.77	0.64
1:D:187:GLN:HG3	3:D:4542:HOH:O	1.98	0.64
1:B:307:ARG:HG2	1:B:307:ARG:HH11	1.61	0.64
1:A:352:ARG:O	1:A:353:GLU:HB2	1.98	0.64
1:D:307:ARG:HD2	3:D:4741:HOH:O	1.97	0.64
1:A:318:ILE:HG22	1:A:319:ARG:N	2.12	0.64
1:C:165:ARG:NH1	3:C:3796:HOH:O	2.29	0.64
1:D:93:LYS:HE2	3:D:4723:HOH:O	1.98	0.63
1:A:364:LEU:HD11	1:A:370:VAL:HG23	1.81	0.63
1:B:73:HIS:CB	1:B:117:ARG:HH12	1.96	0.63
1:D:274:ARG:HB3	3:D:4666:HOH:O	1.98	0.63
1:B:107:LEU:HG	1:B:154:LEU:HD13	1.81	0.63
1:B:178:ASN:HB3	1:B:223:LEU:O	1.99	0.63
1:B:218:HIS:N	3:B:2640:HOH:O	2.26	0.63
1:D:369:VAL:CG2	1:D:389:VAL:HG22	2.29	0.63
1:A:21:MET:HE3	3:A:1615:HOH:O	1.98	0.63
1:B:372:TYR:CG	1:B:394:ALA:HB2	2.34	0.63
1:C:33:THR:CG2	3:C:3691:HOH:O	2.45	0.63
1:D:184:ALA:HA	3:D:4614:HOH:O	1.98	0.63
1:A:44:ASP:OD1	1:A:45:VAL:N	2.32	0.63
1:A:268:ALA:HB1	1:A:301:ILE:CD1	2.29	0.63
1:A:273:SER:OG	1:A:275:ALA:N	2.30	0.63
1:D:107:LEU:HD22	1:D:111:LEU:HD11	1.81	0.62
1:A:43:ASP:O	1:A:44:ASP:HB2	1.98	0.62
1:D:286:CYS:SG	1:D:292:THR:HG23	2.39	0.62
1:A:90:LEU:HB3	1:A:94:ILE:HD12	1.81	0.62
1:A:223:LEU:HD23	1:A:224:GLU:N	2.14	0.62
1:B:183:PRO:HA	1:B:186:ARG:HG3	1.81	0.62
1:B:337:LYS:HB2	1:B:337:LYS:NZ	2.14	0.62
1:A:274:ARG:HG2	1:A:274:ARG:HH11	1.64	0.62
1:A:183:PRO:HA	1:A:186:ARG:CD	2.29	0.62
1:D:17:LEU:HD21	1:D:20:VAL:HG13	1.80	0.62
1:A:241:GLY:O	1:A:242:GLU:HB2	1.98	0.61
1:A:268:ALA:HB1	1:A:301:ILE:HD11	1.81	0.61
1:B:19:LYS:HB3	1:B:412:VAL:HG23	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:THR:HG21	3:B:2617:HOH:O	1.99	0.61
1:D:243:ARG:HG2	3:D:4722:HOH:O	2.00	0.61
1:D:398:GLY:C	1:D:400:GLY:H	2.08	0.61
1:C:359:ASN:HA	3:C:3798:HOH:O	1.99	0.61
1:A:100:GLY:O	1:A:104:THR:HG23	2.00	0.61
1:A:343:THR:OG1	1:A:359:ASN:ND2	2.32	0.61
1:C:336:LYS:HE3	3:C:3787:HOH:O	2.00	0.61
1:A:95:THR:N	3:A:1721:HOH:O	2.33	0.61
1:D:6:THR:N	3:D:4718:HOH:O	2.33	0.61
1:C:331:GLU:HG2	3:C:3728:HOH:O	2.01	0.61
1:A:273:SER:OG	1:A:275:ALA:HB3	2.01	0.61
1:B:271:PRO:HD3	1:C:148:LEU:HD22	1.82	0.61
1:A:157:PRO:HB2	3:A:1709:HOH:O	2.00	0.60
1:C:206:GLU:HB2	3:C:3789:HOH:O	2.00	0.60
1:C:353:GLU:CD	3:C:3801:HOH:O	2.45	0.60
1:C:118:LYS:HD3	3:C:3679:HOH:O	2.00	0.60
1:A:157:PRO:HD2	3:A:1709:HOH:O	2.01	0.60
1:A:268:ALA:CB	1:A:301:ILE:HD11	2.31	0.60
1:B:183:PRO:HA	1:B:186:ARG:CG	2.31	0.60
1:D:107:LEU:HD11	1:D:155:LEU:HD13	1.82	0.60
1:A:128:ALA:HB3	1:A:131:ASP:OD1	2.02	0.60
1:B:135:SER:O	1:B:139:ASN:ND2	2.30	0.60
1:D:119:LEU:HD12	1:D:119:LEU:O	2.01	0.60
1:D:165:ARG:HD2	1:D:405:HIS:O	2.03	0.59
1:A:331:GLU:HG3	1:A:332:SER:N	2.17	0.59
1:A:327:GLU:O	1:A:330:ALA:HB3	2.02	0.59
1:A:277:MET:HE2	3:A:1702:HOH:O	2.02	0.59
1:D:65:ARG:HG3	1:D:65:ARG:NH1	2.17	0.59
1:A:190:LEU:HD23	3:A:1579:HOH:O	2.02	0.59
1:A:269:GLY:HA3	1:D:148:LEU:HD11	1.85	0.59
1:C:303:PRO:HG2	1:C:321:GLU:HB2	1.84	0.59
1:A:222:THR:O	1:A:244:SER:HA	2.03	0.59
1:C:65:ARG:NH1	3:C:3538:HOH:O	2.35	0.59
1:D:166:ASP:O	1:D:180:MET:HE1	2.03	0.59
1:D:307:ARG:HB2	3:D:4741:HOH:O	2.03	0.59
1:A:264:ARG:NH1	1:A:305:SER:OG	2.35	0.59
1:B:400:GLY:O	1:B:401:ARG:HB2	2.03	0.58
1:D:231:ILE:HD12	1:D:232:GLY:N	2.18	0.58
1:A:80:ILE:HD11	1:A:116:PRO:CA	2.33	0.58
1:C:270:LEU:HD11	3:C:3786:HOH:O	2.04	0.58
1:A:64:GLU:N	3:A:1504:HOH:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:THR:OG1	1:C:327:GLU:HG3	2.03	0.58
1:A:174:GLY:HA3	1:A:210:TRP:NE1	2.18	0.58
1:A:103:LEU:HD13	1:A:154:LEU:CD1	2.32	0.58
1:A:277:MET:CE	3:A:1702:HOH:O	2.52	0.58
1:D:18:ARG:HG3	1:D:18:ARG:HH11	1.69	0.58
1:A:63:ARG:NH2	1:A:69:VAL:O	2.37	0.58
1:A:150:HIS:CE1	3:A:1717:HOH:O	2.57	0.58
1:B:284:SER:O	1:B:291:VAL:HA	2.03	0.57
1:C:359:ASN:N	3:C:3785:HOH:O	2.37	0.57
1:A:243:ARG:HE	1:A:276:ALA:HB1	1.68	0.57
1:A:293:VAL:O	1:A:295:PRO:HD3	2.04	0.57
1:A:295:PRO:HG2	1:A:342:GLU:HB3	1.84	0.57
1:B:165:ARG:O	1:B:225:GLY:HA3	2.05	0.57
1:C:140:ILE:HG22	1:C:143:MET:HE1	1.86	0.57
1:D:314:TYR:HD1	1:D:314:TYR:H	1.50	0.57
1:A:75:LEU:HD23	1:A:199:HIS:NE2	2.19	0.57
1:C:20:VAL:HG12	1:C:410:PRO:HA	1.86	0.57
1:D:288:ARG:CB	1:D:416:ILE:HD11	2.35	0.57
1:C:33:THR:HG23	3:C:3691:HOH:O	2.03	0.57
1:D:71:GLU:OE1	1:D:73:HIS:HB2	2.04	0.57
1:A:177:LEU:HD13	1:A:193:THR:OG1	2.05	0.57
1:B:372:TYR:CD2	1:B:394:ALA:HB2	2.40	0.57
1:C:271:PRO:O	1:C:272:LYS:HB3	2.04	0.57
1:D:55:HIS:O	1:D:58:PHE:HB3	2.05	0.57
1:D:87:LYS:NZ	3:D:4641:HOH:O	2.36	0.57
1:D:139:ASN:O	1:D:143:MET:HG3	2.05	0.56
1:A:218:HIS:HB2	3:A:1558:HOH:O	2.05	0.56
1:A:372:TYR:CD2	1:A:394:ALA:HB2	2.39	0.56
1:B:324:THR:OG1	1:B:327:GLU:HG3	2.06	0.56
1:C:56:PHE:HA	3:C:3556:HOH:O	2.03	0.56
1:D:224:GLU:OE1	1:D:278:HIS:NE2	2.37	0.56
1:A:118:LYS:NZ	3:A:1614:HOH:O	2.39	0.56
1:B:140:ILE:HD13	1:C:318:ILE:HG21	1.86	0.56
1:C:370:VAL:HA	1:C:390:ILE:O	2.05	0.56
1:B:277:MET:N	3:B:2769:HOH:O	2.39	0.56
1:C:336:LYS:HG3	3:C:3760:HOH:O	2.05	0.56
1:D:89:ILE:HD11	1:D:194:ALA:CB	2.36	0.56
1:A:206:GLU:O	1:A:207:PHE:HB3	2.05	0.56
1:C:80:ILE:HD12	1:C:119:LEU:HD13	1.86	0.56
1:C:140:ILE:HG22	1:C:143:MET:CE	2.36	0.56
1:C:187:GLN:HE21	1:C:187:GLN:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:GLY:O	1:C:30:GLN:HG3	2.05	0.56
1:C:93:LYS:HE3	1:C:155:LEU:HG	1.87	0.56
1:C:399:ARG:NH2	3:C:3595:HOH:O	2.39	0.56
1:A:130:ASP:HB3	1:A:142:LYS:NZ	2.22	0.56
1:B:227:ASP:O	1:B:238:ILE:HA	2.05	0.56
1:C:33:THR:HG23	1:C:34:PRO:HD2	1.86	0.56
1:D:231:ILE:HD12	1:D:231:ILE:C	2.30	0.56
1:B:344:GLY:C	3:B:2668:HOH:O	2.48	0.55
1:D:374:ARG:NH2	3:D:4738:HOH:O	2.39	0.55
1:C:323:LYS:NZ	3:C:3791:HOH:O	2.39	0.55
1:C:65:ARG:NH2	1:C:390:ILE:HD11	2.20	0.55
1:D:295:PRO:HG3	1:D:342:GLU:HG2	1.88	0.55
1:A:227:ASP:O	1:A:238:ILE:HA	2.06	0.55
1:C:323:LYS:HE2	3:C:3791:HOH:O	2.05	0.55
1:C:372:TYR:CG	1:C:394:ALA:HB2	2.41	0.55
1:D:17:LEU:HD11	1:D:20:VAL:HG13	1.88	0.55
1:B:10:VAL:HG21	1:B:410:PRO:O	2.07	0.55
1:A:273:SER:HB3	3:A:1702:HOH:O	2.05	0.55
1:D:50:GLN:OE1	1:D:53:ARG:NH2	2.37	0.55
1:C:323:LYS:CE	3:C:3791:HOH:O	2.54	0.55
1:D:65:ARG:CG	1:D:65:ARG:NH1	2.64	0.55
1:B:309:ASP:OD2	1:B:311:SER:HB3	2.07	0.55
1:C:101:LEU:HD12	1:C:102:GLY:N	2.21	0.55
1:D:292:THR:OG1	1:D:359:ASN:ND2	2.39	0.55
1:D:343:THR:CG2	1:D:344:GLY:N	2.70	0.55
1:A:156:PRO:CG	1:A:187:GLN:NE2	2.70	0.55
1:B:132:LEU:HD11	1:B:154:LEU:HD11	1.88	0.55
1:B:350:ALA:HB3	1:B:377:TYR:OH	2.06	0.54
1:D:54:ASP:HA	3:D:4731:HOH:O	2.07	0.54
1:C:307:ARG:HH11	1:C:307:ARG:HG2	1.73	0.54
1:B:305:SER:C	1:B:318:ILE:HD12	2.32	0.54
1:C:6:THR:HG23	1:C:6:THR:O	2.07	0.54
1:C:140:ILE:HG13	1:C:141:LEU:N	2.22	0.54
1:D:274:ARG:C	1:D:276:ALA:H	2.15	0.54
1:D:72:MET:HE1	3:D:4504:HOH:O	2.07	0.54
1:A:199:HIS:HE1	1:A:201:GLU:HG3	1.73	0.54
1:A:296:GLU:OE2	1:A:296:GLU:N	2.41	0.54
1:B:165:ARG:CD	1:B:405:HIS:O	2.52	0.54
1:B:350:ALA:C	1:B:351:GLU:HG3	2.31	0.54
1:A:199:HIS:CE1	1:A:201:GLU:HG3	2.42	0.54
1:C:17:LEU:HD21	1:C:20:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:343:THR:HG23	1:D:344:GLY:N	2.23	0.54
1:D:355:TRP:NE1	3:D:4686:HOH:O	2.38	0.54
1:A:266:ILE:HD13	1:A:328:VAL:HG12	1.89	0.54
1:C:304:PHE:CE1	1:C:320:ARG:HG3	2.43	0.54
1:B:38:ASP:HB2	3:B:2577:HOH:O	2.07	0.54
1:B:98:SER:HB2	3:B:2758:HOH:O	2.08	0.54
1:C:165:ARG:O	1:C:225:GLY:HA3	2.06	0.54
1:A:355:TRP:CH2	1:A:357:ASP:HB2	2.43	0.53
1:C:7:LYS:HE2	1:C:206:GLU:OE1	2.08	0.53
1:C:25:PRO:HA	1:C:29:HIS:CE1	2.43	0.53
1:A:148:LEU:HB3	3:A:1717:HOH:O	2.08	0.53
1:C:239:GLY:HA2	1:C:268:ALA:HB3	1.91	0.53
1:A:106:GLU:HG2	3:A:1700:HOH:O	2.08	0.53
1:B:361:VAL:HG22	3:B:2761:HOH:O	2.08	0.53
1:C:7:LYS:HE2	1:C:206:GLU:CD	2.33	0.53
1:B:352:ARG:NH2	3:B:2667:HOH:O	2.41	0.53
1:C:174:GLY:HA3	1:C:210:TRP:CE2	2.44	0.53
1:C:353:GLU:HG2	3:C:3638:HOH:O	2.08	0.53
1:A:318:ILE:CD1	1:D:140:ILE:HD13	2.38	0.53
3:A:1681:HOH:O	1:D:97:ASP:HB3	2.08	0.53
1:B:304:PHE:CB	1:B:318:ILE:HD11	2.32	0.53
1:C:298:VAL:HA	1:C:301:ILE:CD1	2.39	0.53
1:A:254:GLN:NE2	1:A:314:TYR:O	2.42	0.53
1:D:325:PHE:HB3	3:D:4653:HOH:O	2.09	0.53
1:C:204:ASN:HB3	3:C:3716:HOH:O	2.10	0.52
1:A:107:LEU:C	1:A:107:LEU:HD13	2.34	0.52
1:A:358:GLY:HA3	1:A:378:THR:HG21	1.91	0.52
1:B:33:THR:N	1:B:36:ASN:OD1	2.32	0.52
1:D:103:LEU:HD11	1:D:141:LEU:HD23	1.92	0.52
1:D:178:ASN:HB3	1:D:223:LEU:O	2.09	0.52
1:C:307:ARG:HG2	1:C:307:ARG:NH1	2.24	0.52
1:D:22:VAL:HA	1:D:164:THR:HG21	1.91	0.52
1:B:71:GLU:HB3	1:B:74:ASN:HD22	1.73	0.52
1:A:343:THR:HG22	1:A:378:THR:OG1	2.10	0.52
1:C:87:LYS:CE	3:C:3804:HOH:O	2.54	0.52
1:D:355:TRP:CH2	1:D:357:ASP:HB3	2.45	0.52
1:A:71:GLU:OE2	1:A:73:HIS:N	2.29	0.52
1:C:175:VAL:N	3:C:3784:HOH:O	2.43	0.51
1:A:359:ASN:O	1:A:360:ASN:CB	2.58	0.51
1:B:355:TRP:CZ3	1:B:357:ASP:HB2	2.45	0.51
1:C:43:ASP:OD2	1:C:401:ARG:NE	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:C	1:A:80:ILE:HD12	2.35	0.51
1:B:199:HIS:CE1	1:B:201:GLU:HB2	2.46	0.51
1:B:259:LYS:CD	1:B:259:LYS:N	2.73	0.51
1:A:146:GLU:HG3	3:A:1623:HOH:O	2.11	0.51
1:A:344:GLY:HA2	3:A:1670:HOH:O	2.10	0.51
1:C:240:MET:CG	1:C:241:GLY:N	2.71	0.51
1:A:353:GLU:HG2	3:A:1640:HOH:O	2.09	0.51
1:B:14:ALA:C	1:B:366:PRO:HD3	2.28	0.51
1:C:158:LEU:HD21	1:C:187:GLN:HB2	1.93	0.51
1:D:276:ALA:HB2	3:D:4575:HOH:O	2.10	0.51
1:D:312:SER:HB3	1:D:314:TYR:CD1	2.46	0.51
1:A:356:ASP:C	1:A:356:ASP:OD1	2.54	0.51
1:B:72:MET:HE1	3:B:2617:HOH:O	2.11	0.51
1:D:242:GLU:HB2	3:D:4722:HOH:O	2.10	0.51
1:D:299:LYS:HD2	1:D:300:GLU:HG2	1.93	0.51
1:C:84:GLU:HB2	3:C:3705:HOH:O	2.10	0.51
1:D:352:ARG:CZ	1:D:352:ARG:HB2	2.41	0.51
1:A:181:TYR:HD2	1:A:243:ARG:HD3	1.75	0.50
1:B:398:GLY:C	1:B:400:GLY:H	2.19	0.50
1:B:305:SER:O	1:B:318:ILE:HD12	2.11	0.50
1:D:145:ARG:NH2	1:D:146:GLU:HB2	2.27	0.50
1:B:361:VAL:HB	1:B:369:VAL:CG1	2.39	0.50
1:B:363:CYS:HB2	1:B:413:ARG:NH2	2.26	0.50
1:A:374:ARG:NH2	1:B:396:GLU:OE2	2.45	0.50
1:B:31:ARG:HG2	1:B:31:ARG:HH11	1.76	0.50
1:D:284:SER:HG	1:D:292:THR:HG1	1.54	0.50
1:B:165:ARG:HD2	1:B:408:THR:O	2.10	0.50
1:C:8:LEU:HD22	1:C:411:ILE:HG22	1.94	0.50
1:C:33:THR:CG2	1:C:35:SER:H	2.08	0.50
1:C:293:VAL:HG13	1:C:298:VAL:CG2	2.41	0.50
1:A:264:ARG:HD3	1:A:307:ARG:CZ	2.42	0.50
1:B:217:ASP:HA	3:B:2682:HOH:O	2.11	0.50
1:C:227:ASP:O	1:C:238:ILE:HA	2.12	0.50
1:A:286:CYS:SG	1:A:292:THR:HG23	2.52	0.49
1:B:60:THR:HG23	3:B:2772:HOH:O	2.11	0.49
1:D:398:GLY:C	1:D:400:GLY:N	2.70	0.49
1:A:318:ILE:HG22	1:A:319:ARG:H	1.76	0.49
1:B:45:VAL:HG13	3:B:2510:HOH:O	2.13	0.49
1:D:284:SER:OG	1:D:292:THR:OG1	2.27	0.49
1:A:140:ILE:HG13	1:A:141:LEU:N	2.27	0.49
1:D:101:LEU:HG	3:D:4742:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASP:OD1	1:A:145:ARG:NH1	2.27	0.49
1:C:395:SER:HB3	1:D:395:SER:OG	2.12	0.49
1:A:283:PHE:HD1	1:A:293:VAL:HG12	1.77	0.49
1:A:318:ILE:HD11	3:D:4519:HOH:O	2.12	0.49
1:B:403:GLY:O	1:B:407:MET:HG3	2.12	0.49
1:C:380:THR:HG22	3:C:3772:HOH:O	2.12	0.49
1:A:148:LEU:CB	3:A:1717:HOH:O	2.61	0.49
1:A:148:LEU:HD11	1:D:302:VAL:HB	1.94	0.49
1:B:306:LEU:HD13	1:B:318:ILE:HB	1.94	0.49
1:C:187:GLN:HA	1:C:187:GLN:NE2	2.27	0.49
1:C:290:LEU:HD23	1:C:339:ARG:O	2.13	0.49
1:D:87:LYS:CE	3:D:4672:HOH:O	2.61	0.49
1:A:301:ILE:HD13	1:A:325:PHE:CD1	2.47	0.49
1:C:240:MET:HB2	1:C:249:ILE:CD1	2.43	0.49
1:B:320:ARG:NH1	1:B:320:ARG:HG2	2.28	0.49
1:B:337:LYS:HB2	1:B:337:LYS:HZ2	1.78	0.49
1:A:237:LEU:HD21	1:A:329:VAL:HG22	1.95	0.49
1:D:22:VAL:CA	1:D:164:THR:HG21	2.42	0.49
1:B:370:VAL:HA	1:B:390:ILE:O	2.13	0.48
1:C:115:GLU:H	1:C:118:LYS:HE3	1.77	0.48
1:A:240:MET:HE2	1:A:246:ARG:CA	2.42	0.48
1:A:80:ILE:HD11	1:A:116:PRO:HB3	1.94	0.48
1:A:359:ASN:HA	3:A:1646:HOH:O	2.13	0.48
1:B:271:PRO:HD3	1:C:148:LEU:CD2	2.43	0.48
1:B:288:ARG:HG3	1:B:288:ARG:NH1	2.28	0.48
1:D:86:LEU:O	1:D:90:LEU:HG	2.13	0.48
1:D:213:ASP:C	1:D:213:ASP:OD1	2.55	0.48
1:C:166:ASP:HA	1:C:225:GLY:HA3	1.95	0.48
1:D:400:GLY:O	1:D:401:ARG:HB2	2.14	0.48
1:A:16:LYS:HE2	1:A:365:GLU:HG2	1.95	0.48
1:A:295:PRO:CG	1:A:342:GLU:HB3	2.42	0.48
1:B:240:MET:HE1	1:C:144:TYR:CE1	2.48	0.48
1:C:106:GLU:HG2	3:C:3509:HOH:O	2.14	0.48
1:D:18:ARG:HH11	1:D:18:ARG:CG	2.25	0.48
1:D:175:VAL:HG22	1:D:176:THR:N	2.28	0.48
1:A:17:LEU:HD21	1:A:20:VAL:HG13	1.95	0.48
1:A:145:ARG:HG2	1:A:146:GLU:N	2.28	0.48
1:A:257:PHE:CD2	1:A:316:MET:HG2	2.49	0.48
1:C:78:GLU:OE1	1:C:199:HIS:HE1	1.96	0.48
1:D:12:SER:HA	1:D:230:PRO:O	2.14	0.48
1:A:178:ASN:HA	1:A:179:PRO:HD3	1.69	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ILE:HG21	1:B:249:ILE:HG12	1.95	0.48
1:C:187:GLN:HE21	1:C:187:GLN:CA	2.26	0.48
1:C:288:ARG:NH1	1:C:416:ILE:HG23	2.29	0.48
1:D:46:ILE:HG22	1:D:399:ARG:HD2	1.96	0.48
1:B:358:GLY:HA3	1:B:378:THR:HG21	1.96	0.47
1:B:400:GLY:O	2:B:2500:ARG:N	2.47	0.47
1:C:17:LEU:HD13	1:C:413:ARG:NH2	2.29	0.47
1:D:330:ALA:O	1:D:335:LEU:HB2	2.14	0.47
1:A:29:HIS:HE1	3:A:1653:HOH:O	1.98	0.47
1:A:193:THR:HG21	1:A:214:PRO:HG3	1.96	0.47
1:B:165:ARG:NH2	3:B:2522:HOH:O	2.46	0.47
1:C:174:GLY:HA3	1:C:210:TRP:NE1	2.29	0.47
1:B:170:TRP:CD1	1:B:170:TRP:N	2.82	0.47
1:B:254:GLN:NE2	1:C:101:LEU:HD22	2.28	0.47
1:C:248:ALA:O	1:C:252:VAL:HG23	2.14	0.47
1:B:47:TRP:CD2	1:B:50:GLN:HB2	2.50	0.47
1:C:336:LYS:HE2	1:C:336:LYS:HB3	1.79	0.47
1:D:78:GLU:HA	1:D:81:GLN:HG3	1.96	0.47
1:D:222:THR:O	1:D:244:SER:HA	2.15	0.47
1:A:45:VAL:HG12	1:A:46:ILE:N	2.30	0.47
1:A:46:ILE:HG22	1:A:399:ARG:HD2	1.97	0.47
1:A:129:ALA:HB3	3:A:1647:HOH:O	2.15	0.47
1:C:82:ASN:C	1:C:82:ASN:OD1	2.57	0.47
1:C:354:GLN:HE22	1:D:47:TRP:CA	2.15	0.47
1:C:380:THR:HG23	3:C:3564:HOH:O	2.15	0.47
1:D:107:LEU:HD11	1:D:155:LEU:CD1	2.44	0.47
1:A:178:ASN:HB2	1:A:180:MET:HE1	1.95	0.47
1:A:202:PHE:O	1:A:205:ALA:HB3	2.15	0.47
1:C:62:MET:CG	1:C:67:ILE:HD12	2.45	0.47
1:D:287:ASP:HB3	1:D:290:LEU:HB2	1.96	0.47
1:C:62:MET:HG3	1:C:67:ILE:HD12	1.96	0.47
1:D:293:VAL:O	1:D:295:PRO:HD3	2.14	0.47
1:A:231:ILE:HD12	1:A:333:LEU:HD23	1.96	0.46
1:A:301:ILE:HG12	1:A:302:VAL:N	2.28	0.46
1:D:11:HIS:HB2	1:D:415:PRO:HD3	1.97	0.46
1:A:144:TYR:CE1	1:D:240:MET:HE1	2.51	0.46
1:A:275:ALA:HB3	3:A:1619:HOH:O	2.16	0.46
1:B:167:THR:HG23	3:B:2519:HOH:O	2.15	0.46
1:D:160:ASN:C	1:D:162:GLN:N	2.71	0.46
1:A:88:TRP:O	1:A:92:ARG:HD2	2.14	0.46
1:B:288:ARG:NH1	1:B:288:ARG:CG	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:SER:OG	1:A:247:GLN:HB3	2.15	0.46
1:B:31:ARG:HD2	1:B:157:PRO:HB3	1.98	0.46
1:B:97:ASP:O	1:C:220:SER:HB2	2.15	0.46
1:B:98:SER:CA	3:B:2758:HOH:O	2.63	0.46
1:C:175:VAL:CG1	3:C:3784:HOH:O	2.60	0.46
1:D:380:THR:O	1:D:384:LYS:HG2	2.16	0.46
1:B:103:LEU:HD13	1:B:154:LEU:HD21	1.97	0.46
1:D:87:LYS:O	1:D:91:ASP:HB2	2.15	0.46
1:B:63:ARG:C	1:B:65:ARG:N	2.73	0.46
1:D:370:VAL:HA	1:D:390:ILE:O	2.16	0.46
1:C:33:THR:HG23	1:C:34:PRO:CD	2.46	0.46
1:C:299:LYS:NZ	1:C:299:LYS:HB3	2.31	0.46
1:A:94:ILE:HG23	3:A:1721:HOH:O	2.13	0.46
1:A:99:VAL:HG13	1:A:154:LEU:HD12	1.98	0.46
1:C:416:ILE:HG22	1:C:417:ASP:N	2.31	0.46
1:D:208:GLU:OE1	1:D:259:LYS:HE3	2.15	0.46
1:B:9:GLY:HA2	1:B:172:TYR:O	2.16	0.45
1:B:71:GLU:HB3	1:B:74:ASN:ND2	2.30	0.45
1:D:165:ARG:O	1:D:225:GLY:HA3	2.16	0.45
1:A:14:ALA:HB3	1:A:416:ILE:HD11	1.98	0.45
1:A:17:LEU:HD21	1:A:20:VAL:CG1	2.46	0.45
1:A:80:ILE:HD11	1:A:116:PRO:CB	2.46	0.45
1:A:139:ASN:HB3	3:A:1631:HOH:O	2.15	0.45
1:A:240:MET:HG2	1:A:241:GLY:N	2.30	0.45
1:C:229:MET:HB2	1:C:237:LEU:HB2	1.98	0.45
1:D:277:MET:CG	3:D:4727:HOH:O	2.64	0.45
1:D:344:GLY:N	1:D:356:ASP:O	2.46	0.45
1:A:354:GLN:HE22	1:B:47:TRP:HA	1.80	0.45
1:B:272:LYS:HD2	1:B:272:LYS:HA	1.61	0.45
1:C:24:SER:HA	1:C:55:HIS:CD2	2.51	0.45
1:C:61:LYS:HD3	1:C:390:ILE:CG2	2.45	0.45
1:C:331:GLU:CG	3:C:3728:HOH:O	2.60	0.45
1:D:28:ALA:HB2	1:D:125:GLY:HA2	1.98	0.45
1:A:180:MET:HG3	1:A:185:ARG:O	2.16	0.45
1:B:217:ASP:O	1:B:217:ASP:OD1	2.34	0.45
1:C:7:LYS:HG2	1:C:206:GLU:CG	2.46	0.45
1:C:33:THR:CG2	1:C:34:PRO:N	2.79	0.45
1:A:166:ASP:O	1:A:180:MET:HE1	2.16	0.45
1:A:242:GLU:OE1	1:A:272:LYS:HD3	2.17	0.45
1:C:154:LEU:N	1:C:154:LEU:HD22	2.31	0.45
1:A:318:ILE:CG2	1:A:319:ARG:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ASP:C	1:D:215:ASP:H	2.24	0.45
1:D:381:LEU:N	1:D:381:LEU:HD23	2.32	0.45
1:A:94:ILE:C	3:A:1721:HOH:O	2.58	0.45
1:A:156:PRO:CD	1:A:187:GLN:HE22	2.30	0.45
1:A:355:TRP:HH2	3:B:2764:HOH:O	1.99	0.45
1:B:320:ARG:HG2	1:B:320:ARG:HH11	1.83	0.45
1:A:145:ARG:NH1	3:A:1647:HOH:O	2.49	0.44
1:A:290:LEU:HD22	1:A:291:VAL:N	2.31	0.44
1:D:231:ILE:HD13	1:D:333:LEU:HD23	1.96	0.44
1:A:156:PRO:HG3	1:A:187:GLN:HE22	1.80	0.44
1:B:11:HIS:HB2	1:B:415:PRO:HB3	1.99	0.44
1:B:71:GLU:HG3	1:B:74:ASN:H	1.82	0.44
1:C:200:PRO:HA	3:C:3704:HOH:O	2.16	0.44
1:B:108:ARG:O	1:B:112:GLU:HG3	2.18	0.44
1:C:280:ASP:HA	1:C:283:PHE:O	2.18	0.44
1:D:8:LEU:HA	1:D:412:VAL:HG22	1.98	0.44
1:A:374:ARG:NH2	1:B:399:ARG:CZ	2.80	0.44
1:D:256:LEU:HB2	3:D:4747:HOH:O	2.18	0.44
1:C:199:HIS:HD2	1:C:201:GLU:N	1.94	0.44
1:D:246:ARG:HG3	1:D:247:GLN:N	2.33	0.44
1:B:183:PRO:HA	1:B:186:ARG:HG2	2.00	0.44
1:B:307:ARG:HG2	1:B:307:ARG:NH1	2.31	0.44
1:A:275:ALA:CB	3:A:1619:HOH:O	2.65	0.44
1:B:148:LEU:HD11	1:C:302:VAL:HB	2.00	0.44
1:B:180:MET:O	1:B:186:ARG:NE	2.50	0.44
1:D:177:LEU:N	1:D:177:LEU:HD23	2.32	0.44
1:A:73:HIS:CD2	1:A:124:ILE:HD12	2.53	0.44
1:C:298:VAL:HA	1:C:301:ILE:HD12	2.00	0.44
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.89	0.44
1:B:187:GLN:HG3	3:B:2604:HOH:O	2.17	0.44
1:D:75:LEU:HD23	3:D:4640:HOH:O	2.18	0.44
1:D:374:ARG:CZ	3:D:4738:HOH:O	2.66	0.44
1:B:242:GLU:HB2	3:B:2562:HOH:O	2.18	0.43
1:B:257:PHE:CG	1:B:308:PRO:HG3	2.52	0.43
1:B:343:THR:HG22	1:B:378:THR:OG1	2.17	0.43
1:B:350:ALA:CB	1:B:377:TYR:OH	2.65	0.43
1:C:306:LEU:HA	1:C:317:ASN:O	2.18	0.43
1:D:355:TRP:CZ3	1:D:357:ASP:CG	2.96	0.43
1:A:170:TRP:CE2	1:A:411:ILE:HG23	2.53	0.43
1:A:240:MET:CG	1:A:241:GLY:N	2.80	0.43
1:B:98:SER:HA	3:B:2758:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:HIS:CE1	1:C:241:GLY:HA3	2.53	0.43
1:B:309:ASP:O	1:B:315:GLY:HA2	2.18	0.43
1:C:87:LYS:NZ	3:C:3804:HOH:O	2.49	0.43
1:A:207:PHE:CD1	1:A:207:PHE:C	2.95	0.43
1:A:414:ASP:HA	1:A:415:PRO:HD3	1.81	0.43
1:B:57:ASP:CG	1:B:61:LYS:HE3	2.43	0.43
1:B:281:THR:O	1:B:281:THR:CG2	2.65	0.43
1:C:167:THR:HG21	3:C:3644:HOH:O	2.17	0.43
1:D:82:ASN:OD1	1:D:82:ASN:C	2.61	0.43
1:D:264:ARG:CZ	1:D:266:ILE:HD11	2.48	0.43
1:D:273:SER:O	1:D:273:SER:OG	2.31	0.43
1:D:302:VAL:HA	1:D:303:PRO:HD3	1.78	0.43
1:A:55:HIS:O	1:A:58:PHE:HB3	2.19	0.43
1:A:213:ASP:OD1	1:A:215:ASP:HB2	2.19	0.43
1:B:41:LEU:HD13	2:B:2500:ARG:OXT	2.19	0.43
1:C:298:VAL:HG13	1:C:301:ILE:HD12	2.01	0.43
1:A:99:VAL:CG1	1:A:154:LEU:HD12	2.48	0.43
1:B:20:VAL:HG12	1:B:410:PRO:HA	1.99	0.43
1:B:98:SER:CB	3:B:2758:HOH:O	2.66	0.43
1:C:361:VAL:HG21	1:C:369:VAL:HG21	1.99	0.43
1:D:309:ASP:N	1:D:316:MET:HA	2.33	0.43
1:A:356:ASP:HB2	3:A:1621:HOH:O	2.18	0.43
1:B:80:ILE:HD12	1:B:120:ALA:HB2	1.99	0.43
1:C:140:ILE:HA	1:C:143:MET:HB2	2.00	0.43
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.94	0.43
1:C:17:LEU:HD13	1:C:413:ARG:CZ	2.49	0.43
1:A:240:MET:CB	3:A:1703:HOH:O	2.60	0.43
1:A:292:THR:HA	1:A:341:VAL:O	2.18	0.43
1:A:413:ARG:NH1	3:A:1522:HOH:O	2.37	0.43
1:C:312:SER:HA	1:C:313:PRO:HD3	1.75	0.43
1:C:341:VAL:HG21	1:C:382:LEU:CD1	2.49	0.43
1:D:314:TYR:HD1	1:D:314:TYR:N	2.16	0.43
1:A:397:LEU:HD12	1:A:397:LEU:HA	1.85	0.43
1:B:178:ASN:OD1	1:B:223:LEU:HD13	2.18	0.43
1:D:362:VAL:HG13	1:D:362:VAL:O	2.17	0.43
1:A:140:ILE:O	1:A:143:MET:HB3	2.19	0.43
1:A:157:PRO:O	3:A:1709:HOH:O	2.21	0.43
1:A:213:ASP:HA	1:A:214:PRO:HD2	1.74	0.43
1:B:259:LYS:HD3	1:B:259:LYS:N	2.34	0.43
1:B:351:GLU:HA	3:B:2665:HOH:O	2.18	0.43
1:D:80:ILE:HG23	1:D:86:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:MET:HG2	1:D:185:ARG:HB3	2.01	0.43
1:A:324:THR:O	1:A:325:PHE:C	2.62	0.42
1:A:337:LYS:HE2	3:A:1711:HOH:O	2.19	0.42
1:C:400:GLY:O	1:C:401:ARG:HB2	2.19	0.42
1:C:364:LEU:HD11	1:C:370:VAL:CG2	2.49	0.42
1:D:167:THR:HG22	1:D:168:THR:HG23	2.00	0.42
1:D:217:ASP:C	1:D:219:GLY:H	2.27	0.42
1:D:309:ASP:H	1:D:316:MET:HA	1.84	0.42
1:C:355:TRP:CZ3	1:C:357:ASP:HB2	2.54	0.42
1:D:18:ARG:HB2	1:D:412:VAL:HG12	2.02	0.42
1:A:82:ASN:OD1	1:A:82:ASN:C	2.62	0.42
1:A:309:ASP:HB2	1:A:317:ASN:ND2	2.34	0.42
1:B:38:ASP:HB3	3:B:2572:HOH:O	2.20	0.42
1:B:125:GLY:C	1:B:157:PRO:HA	2.44	0.42
1:C:187:GLN:NE2	1:C:187:GLN:CA	2.82	0.42
1:D:144:TYR:O	1:D:148:LEU:HB2	2.19	0.42
1:A:156:PRO:CG	1:A:187:GLN:HE22	2.32	0.42
1:B:101:LEU:CD1	1:B:101:LEU:N	2.71	0.42
1:B:223:LEU:HD22	1:B:224:GLU:N	2.35	0.42
1:C:62:MET:HB3	1:C:69:VAL:HG21	2.00	0.42
1:D:148:LEU:HD13	1:D:150:HIS:CE1	2.54	0.42
1:D:365:GLU:O	1:D:366:PRO:C	2.60	0.42
1:B:119:LEU:HD23	1:B:123:LEU:HG	2.00	0.42
1:A:272:LYS:HD2	1:A:273:SER:H	1.85	0.42
1:A:352:ARG:N	3:A:1710:HOH:O	2.52	0.42
1:B:370:VAL:HG22	1:B:390:ILE:HB	2.01	0.42
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.84	0.42
1:B:57:ASP:OD1	1:B:61:LYS:HE3	2.20	0.42
1:C:65:ARG:HG3	1:C:65:ARG:HH11	1.84	0.42
1:D:76:LEU:HD22	1:D:80:ILE:CD1	2.42	0.42
1:D:152:SER:CB	3:D:4734:HOH:O	2.67	0.42
1:A:238:ILE:CG2	1:A:249:ILE:HG12	2.43	0.42
1:A:331:GLU:C	1:A:333:LEU:N	2.78	0.42
1:C:47:TRP:CD2	1:C:50:GLN:HB2	2.54	0.42
1:D:27:LEU:HA	1:D:30:GLN:NE2	2.34	0.42
1:A:76:LEU:O	1:A:79:THR:HB	2.20	0.42
1:A:257:PHE:HD2	1:A:316:MET:HG2	1.85	0.42
1:A:273:SER:O	1:A:274:ARG:C	2.60	0.42
1:D:9:GLY:HA2	1:D:172:TYR:O	2.20	0.42
1:D:374:ARG:NE	3:D:4738:HOH:O	2.52	0.42
1:B:398:GLY:C	1:B:400:GLY:N	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:TYR:CG	1:D:394:ALA:HB2	2.55	0.41
1:C:18:ARG:NH1	3:C:3642:HOH:O	2.53	0.41
1:C:359:ASN:HB2	3:C:3785:HOH:O	2.18	0.41
1:D:53:ARG:NH2	3:D:4501:HOH:O	2.46	0.41
1:D:152:SER:HB2	3:D:4734:HOH:O	2.18	0.41
1:D:165:ARG:HB2	1:D:408:THR:O	2.20	0.41
1:D:323:LYS:HG2	1:D:327:GLU:CB	2.38	0.41
1:C:279:LEU:CA	3:C:3786:HOH:O	2.59	0.41
1:D:119:LEU:HD12	1:D:123:LEU:HG	2.02	0.41
1:A:320:ARG:NH2	1:A:322:GLU:OE1	2.53	0.41
1:B:279:LEU:C	1:B:281:THR:H	2.29	0.41
1:D:208:GLU:HG2	1:D:210:TRP:CZ3	2.55	0.41
1:A:359:ASN:O	1:A:360:ASN:HB2	2.19	0.41
1:B:86:LEU:HA	1:B:86:LEU:HD23	1.72	0.41
1:B:305:SER:O	1:B:318:ILE:HA	2.21	0.41
1:D:71:GLU:CD	1:D:73:HIS:H	2.27	0.41
1:A:239:GLY:HA2	1:A:268:ALA:HB3	2.01	0.41
1:C:213:ASP:OD1	1:C:215:ASP:HB2	2.21	0.41
1:C:158:LEU:CD2	1:C:187:GLN:HB2	2.51	0.41
1:D:312:SER:HB3	1:D:314:TYR:CE1	2.56	0.41
1:C:58:PHE:CE1	1:C:370:VAL:HG11	2.56	0.41
1:D:291:VAL:HG22	1:D:340:VAL:HG12	2.03	0.41
1:D:343:THR:HG23	1:D:344:GLY:H	1.86	0.41
1:A:193:THR:O	1:A:197:LYS:HB2	2.21	0.41
1:A:274:ARG:HG2	1:A:274:ARG:NH1	2.32	0.41
1:A:324:THR:O	1:A:327:GLU:N	2.54	0.41
1:B:128:ALA:O	1:B:129:ALA:C	2.63	0.41
1:B:147:TYR:HB3	1:C:302:VAL:HG21	2.01	0.41
1:B:160:ASN:C	1:B:162:GLN:N	2.77	0.41
1:B:272:LYS:HD2	1:B:273:SER:H	1.85	0.41
1:C:64:GLU:CG	3:C:3618:HOH:O	2.69	0.41
1:C:180:MET:HA	1:C:180:MET:CE	2.45	0.41
1:D:145:ARG:HH21	1:D:146:GLU:HB2	1.86	0.41
1:D:317:ASN:O	3:D:4741:HOH:O	2.22	0.41
1:A:11:HIS:O	1:A:12:SER:HB3	2.21	0.41
1:A:318:ILE:HB	1:D:140:ILE:HD13	2.03	0.41
1:D:253:ALA:HA	3:D:4747:HOH:O	2.21	0.41
1:D:268:ALA:HB2	1:D:325:PHE:CE1	2.55	0.41
1:A:146:GLU:CG	3:A:1623:HOH:O	2.69	0.40
1:C:86:LEU:HD22	1:C:90:LEU:HG	2.03	0.40
1:C:133:PRO:O	1:C:134:ALA:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:PRO:O	1:D:299:LYS:HG3	2.21	0.40
1:D:303:PRO:HB2	1:D:321:GLU:HB2	2.03	0.40
1:A:115:GLU:H	1:A:115:GLU:HG2	1.66	0.40
1:B:216:LYS:HG2	1:B:217:ASP:N	2.37	0.40
1:C:180:MET:HB2	1:C:186:ARG:HG2	2.03	0.40
1:D:84:GLU:HG2	1:D:198:PHE:HE1	1.87	0.40
1:D:212:GLY:O	1:D:213:ASP:HB2	2.20	0.40
1:D:307:ARG:HG2	1:D:307:ARG:HH11	1.86	0.40
1:B:67:ILE:H	1:B:67:ILE:HG13	1.72	0.40
1:C:293:VAL:CG1	1:C:294:PHE:N	2.83	0.40
1:C:299:LYS:CE	3:C:3729:HOH:O	2.68	0.40
1:D:46:ILE:HG22	1:D:399:ARG:CD	2.50	0.40
1:A:9:GLY:O	1:A:412:VAL:HA	2.21	0.40
1:A:33:THR:HG22	1:A:36:ASN:OD1	2.21	0.40
1:A:55:HIS:O	1:A:59:VAL:HG23	2.21	0.40
1:D:213:ASP:C	1:D:215:ASP:N	2.79	0.40
1:D:206:GLU:HA	3:D:4584:HOH:O	2.22	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	401/418 (96%)	366 (91%)	27 (7%)	8 (2%)	6	5
1	B	399/418 (96%)	367 (92%)	30 (8%)	2 (0%)	24	31
1	C	396/418 (95%)	368 (93%)	26 (7%)	2 (0%)	24	31
1	D	402/418 (96%)	363 (90%)	32 (8%)	7 (2%)	7	7
All	All	1598/1672 (96%)	1464 (92%)	115 (7%)	19 (1%)	10	12

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	242	GLU
1	B	352	ARG
1	A	273	SER
1	A	353	GLU
1	B	351	GLU
1	D	273	SER
1	D	275	ALA
1	D	296	GLU
1	D	360	ASN
1	A	12	SER
1	A	172	TYR
1	A	360	ASN
1	D	213	ASP
1	D	277	MET
1	A	207	PHE
1	D	101	LEU
1	C	416	ILE
1	C	295	PRO
1	A	230	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/354 (97%)	309 (90%)	35 (10%)	7	8
1	B	344/354 (97%)	312 (91%)	32 (9%)	8	11
1	C	342/354 (97%)	304 (89%)	38 (11%)	6	7
1	D	344/354 (97%)	307 (89%)	37 (11%)	6	7
All	All	1374/1416 (97%)	1232 (90%)	142 (10%)	7	8

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	16	LYS
1	A	20	VAL

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Mol	Chain	Res	Type
1	A	25	PRO
1	A	39	GLU
1	A	40	LEU
1	A	76	LEU
1	A	109	SER
1	A	113	SER
1	A	115	GLU
1	A	119	LEU
1	A	130	ASP
1	A	145	ARG
1	A	155	LEU
1	A	189	THR
1	A	197	LYS
1	A	208	GLU
1	A	223	LEU
1	A	233	ASN
1	A	242	GLU
1	A	272	LYS
1	A	273	SER
1	A	290	LEU
1	A	301	ILE
1	A	319	ARG
1	A	323	LYS
1	A	333	LEU
1	A	352	ARG
1	A	356	ASP
1	A	360	ASN
1	A	369	VAL
1	A	378	THR
1	A	380	THR
1	A	382	LEU
1	A	397	LEU
1	B	20	VAL
1	B	38	ASP
1	B	40	LEU
1	B	64	GLU
1	B	76	LEU
1	B	86	LEU
1	B	101	LEU
1	B	107	LEU
1	B	141	LEU
1	B	167	THR

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Mol	Chain	Res	Type
1	B	208	GLU
1	B	217	ASP
1	B	223	LEU
1	B	247	GLN
1	B	259	LYS
1	B	271	PRO
1	B	272	LYS
1	B	274	ARG
1	B	281	THR
1	B	293	VAL
1	B	307	ARG
1	B	317	ASN
1	B	319	ARG
1	B	331	GLU
1	B	337	LYS
1	B	351	GLU
1	B	356	ASP
1	B	360	ASN
1	B	369	VAL
1	B	382	LEU
1	B	397	LEU
1	B	416	ILE
1	C	20	VAL
1	C	25	PRO
1	C	33	THR
1	C	34	PRO
1	C	38	ASP
1	C	40	LEU
1	C	48	VAL
1	C	62	MET
1	C	64	GLU
1	C	65	ARG
1	C	76	LEU
1	C	86	LEU
1	C	101	LEU
1	C	107	LEU
1	C	119	LEU
1	C	133	PRO
1	C	141	LEU
1	C	143	MET
1	C	155	LEU
1	C	167	THR

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Mol	Chain	Res	Type
1	C	180	MET
1	C	193	THR
1	C	206	GLU
1	C	223	LEU
1	C	259	LYS
1	C	290	LEU
1	C	299	LYS
1	C	323	LYS
1	C	336	LYS
1	C	337	LYS
1	C	352	ARG
1	C	353	GLU
1	C	356	ASP
1	C	360	ASN
1	C	369	VAL
1	C	374	ARG
1	C	382	LEU
1	C	397	LEU
1	D	20	VAL
1	D	40	LEU
1	D	63	ARG
1	D	74	ASN
1	D	76	LEU
1	D	84	GLU
1	D	86	LEU
1	D	107	LEU
1	D	113	SER
1	D	115	GLU
1	D	116	PRO
1	D	118	LYS
1	D	119	LEU
1	D	130	ASP
1	D	165	ARG
1	D	180	MET
1	D	214	PRO
1	D	223	LEU
1	D	235	VAL
1	D	264	ARG
1	D	272	LYS
1	D	273	SER
1	D	274	ARG
1	D	277	MET

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Mol	Chain	Res	Type
1	D	290	LEU
1	D	293	VAL
1	D	311	SER
1	D	312	SER
1	D	313	PRO
1	D	314	TYR
1	D	323	LYS
1	D	331	GLU
1	D	343	THR
1	D	357	ASP
1	D	381	LEU
1	D	397	LEU
1	D	415	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	B	74	ASN
1	B	160	ASN
1	B	254	GLN
1	B	359	ASN
1	C	55	HIS
1	C	187	GLN
1	C	199	HIS
1	C	354	GLN
1	D	29	HIS
1	D	30	GLN
1	D	139	ASN
1	D	199	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ARG	D	4500	-	10,11,11	0.80	0	9,13,13	0.26	0
2	ARG	C	3500	-	10,11,11	0.77	0	9,13,13	0.74	0
2	ARG	B	2500	-	10,11,11	0.66	0	9,13,13	0.75	0
2	ARG	A	1500	-	10,11,11	0.72	0	9,13,13	0.88	1 (11%)

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	ARG	D	4500	-	-	0/11/11/11	-
2	ARG	C	3500	-	-	0/11/11/11	-
2	ARG	B	2500	-	-	1/11/11/11	-
2	ARG	A	1500	-	-	0/11/11/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ARG	OXT-C-O	-2.00	119.54	124.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2500	ARG	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2500	ARG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	405/418 (96%)	-0.46	0 100 100	21, 38, 63, 78	0
1	B	405/418 (96%)	-0.67	1 (0%) 91 91	18, 30, 54, 78	0
1	C	402/418 (96%)	-0.68	0 100 100	18, 30, 54, 74	0
1	D	406/418 (97%)	-0.48	0 100 100	20, 36, 62, 79	0
All	All	1618/1672 (96%)	-0.57	1 (0%) 92 91	18, 33, 60, 79	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	SER	2.3

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	ARG	D	4500	12/12	0.96	0.05	16,28,37,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ARG	B	2500	12/12	0.97	0.04	16,23,26,32	0
2	ARG	C	3500	12/12	0.97	0.05	16,21,29,33	0
2	ARG	A	1500	12/12	0.97	0.05	16,28,39,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.