



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:27 PM UTC

PDB ID : 1GKR / pdb_00001gkr
Title : L-Hydantoinase (Dihydropyrimidinase) from *Arthrobacter aurescens*
Authors : Abendroth, J.; Niefind, K.; Schomburg, D.
Deposited on : 2001-08-20
Resolution : 2.60 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

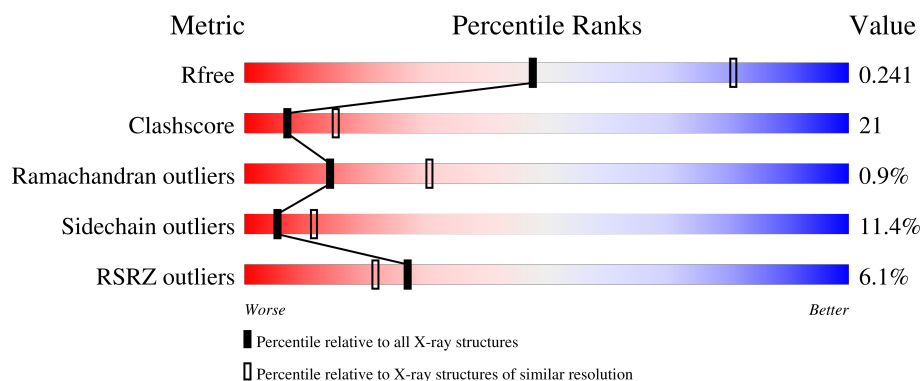
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	458	7% 61% 30% 7% ..
1	B	458	7% 60% 31% 7% ..
1	C	458	7% 60% 31% 7% ..
1	D	458	3% 60% 31% 7% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14196 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 NON-ATP DEPENDENT L-SELECTIVE HYDANTOINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3420	2153	580	666	21			
1	B	451	Total	C	N	O	S	0	0	0
			3420	2153	580	666	21			
1	C	451	Total	C	N	O	S	0	0	0
			3420	2153	580	666	21			
1	D	451	Total	C	N	O	S	0	0	0
			3420	2153	580	666	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	KCX	LYS	modified residue	UNP P81006
B	147	KCX	LYS	modified residue	UNP P81006
C	147	KCX	LYS	modified residue	UNP P81006
D	147	KCX	LYS	modified residue	UNP P81006

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

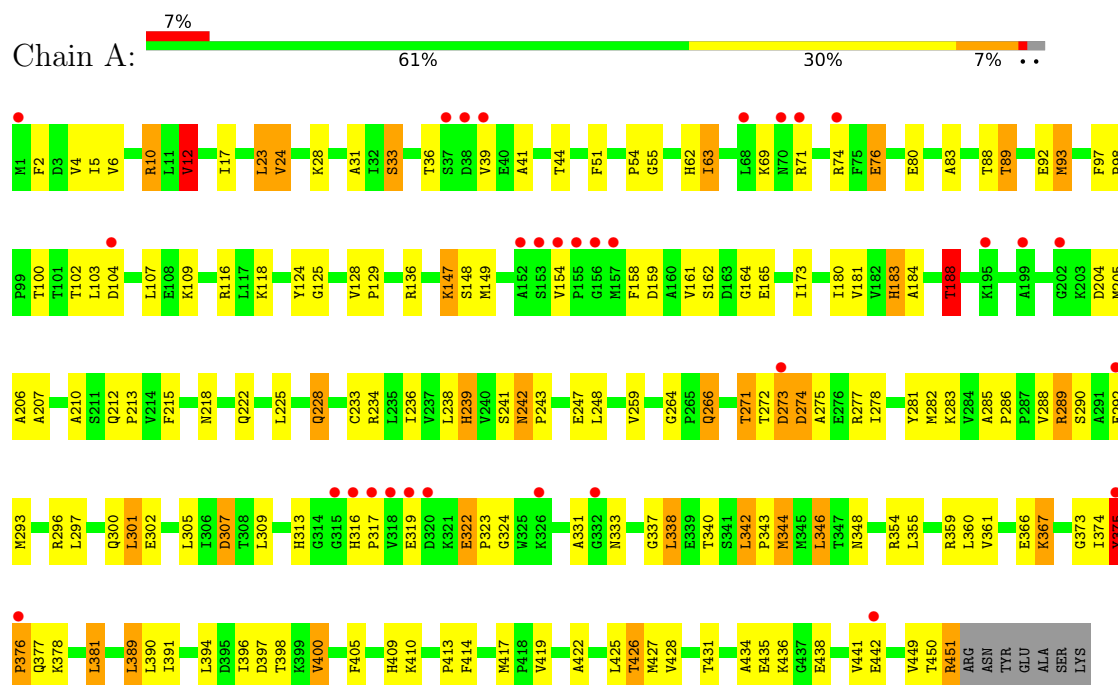
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total 124	O 124	0	0
3	B	129	Total 129	O 129	0	0
3	C	128	Total 128	O 128	0	0
3	D	127	Total 127	O 127	0	0

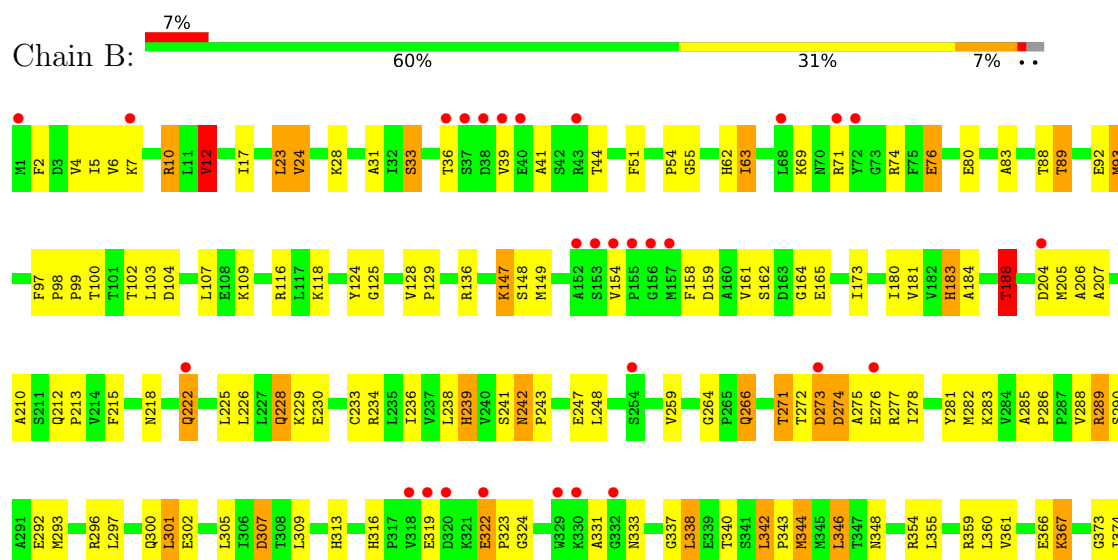
3 Residue-property plots

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: NON-ATP DEPENDENT L-SELECTIVE HYDANTOINASE

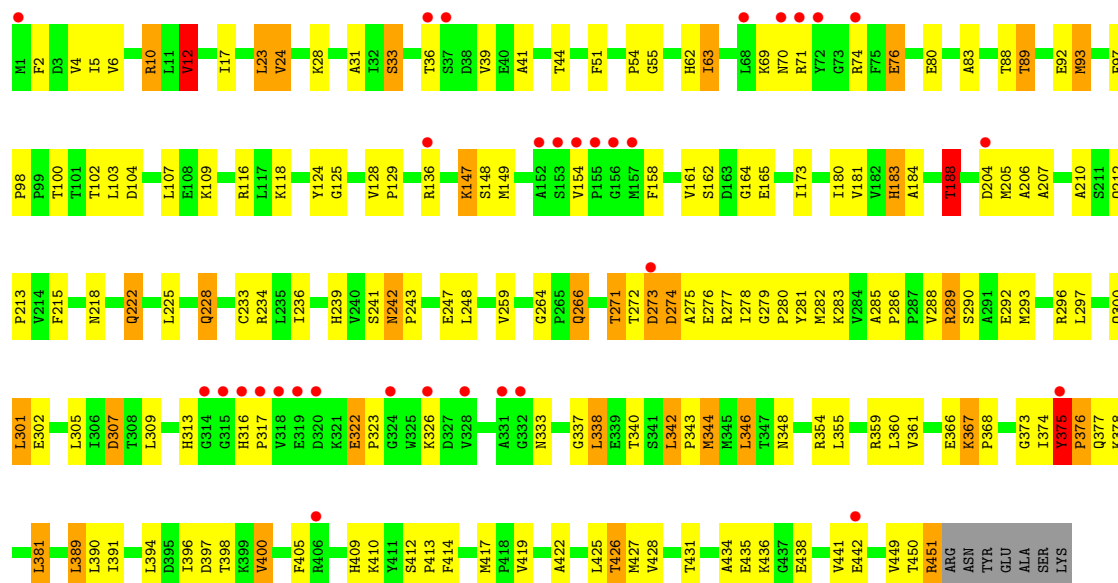


• Molecule 1: NON-ATP DEPENDENT L-SELECTIVE HYDANTOINASE

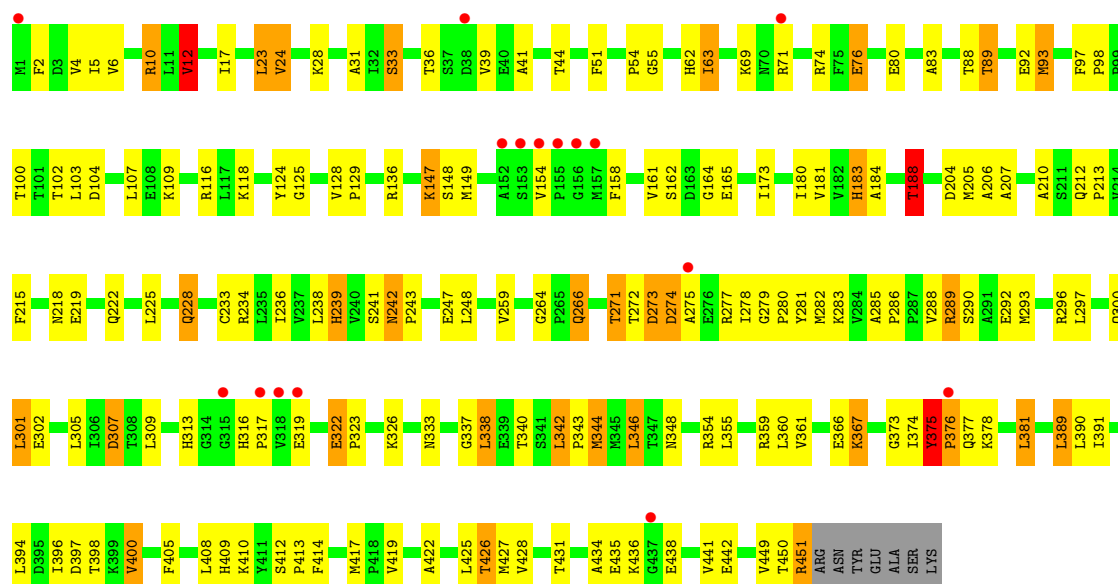




● Molecule 1: NON-ATP DEPENDENT L-SELECTIVE HYDANTOINASE



● Molecule 1: NON-ATP DEPENDENT L-SELECTIVE HYDANTOINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.50Å 74.30Å 146.90Å 90.00° 106.57° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 30.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.3 (30.00-2.60) 86.5 (30.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.244 0.221 , 0.241	Depositor DCC
R_{free} test set	3105 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14196	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.55	0/3466	1.12	23/4689 (0.5%)
1	B	0.55	0/3466	1.12	24/4689 (0.5%)
1	C	0.55	0/3466	1.12	24/4689 (0.5%)
1	D	0.55	0/3466	1.12	23/4689 (0.5%)
All	All	0.55	0/13864	1.12	94/18756 (0.5%)

There are no bond length outliers.

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	MET	N-CA-C	-12.14	96.99	112.90
1	C	205	MET	N-CA-C	-12.14	96.99	112.90
1	B	205	MET	N-CA-C	-12.14	97.00	112.90
1	D	205	MET	N-CA-C	-12.14	97.00	112.90
1	D	274	ASP	N-CA-C	-7.63	103.51	114.12
1	A	274	ASP	N-CA-C	-7.61	103.54	114.12
1	C	274	ASP	N-CA-C	-7.61	103.54	114.12
1	B	274	ASP	N-CA-C	-7.59	103.57	114.12
1	B	125	GLY	N-CA-C	-6.66	99.98	112.10
1	A	125	GLY	N-CA-C	-6.65	99.99	112.10
1	C	125	GLY	N-CA-C	-6.64	100.01	112.10
1	D	125	GLY	N-CA-C	-6.64	100.02	112.10
1	D	366	GLU	N-CA-C	6.61	118.18	110.97
1	A	366	GLU	N-CA-C	6.61	118.17	110.97
1	C	366	GLU	N-CA-C	6.60	118.16	110.97
1	B	366	GLU	N-CA-C	6.58	118.14	110.97
1	D	307	ASP	N-CA-C	6.55	118.50	111.36
1	A	307	ASP	N-CA-C	6.54	118.49	111.36
1	C	307	ASP	N-CA-C	6.52	118.47	111.36
1	B	307	ASP	N-CA-C	6.50	118.44	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	TYR	N-CA-C	6.46	124.08	109.81
1	B	375	TYR	N-CA-C	6.46	124.08	109.81
1	D	375	TYR	N-CA-C	6.45	124.07	109.81
1	C	375	TYR	N-CA-C	6.45	124.06	109.81
1	B	10	ARG	N-CA-C	-6.38	96.24	107.73
1	A	10	ARG	N-CA-C	-6.37	96.27	107.73
1	D	10	ARG	N-CA-C	-6.36	96.28	107.73
1	C	10	ARG	N-CA-C	-6.36	96.28	107.73
1	B	391	ILE	N-CA-C	-5.99	99.24	107.99
1	A	391	ILE	N-CA-C	-5.99	99.25	107.99
1	C	391	ILE	N-CA-C	-5.97	99.27	107.99
1	D	391	ILE	N-CA-C	-5.96	99.29	107.99
1	C	184	ALA	N-CA-C	5.80	118.53	107.75
1	B	184	ALA	N-CA-C	5.79	118.52	107.75
1	A	184	ALA	N-CA-C	5.78	118.50	107.75
1	D	184	ALA	N-CA-C	5.75	118.45	107.75
1	C	288	VAL	N-CA-C	-5.69	102.24	109.58
1	A	288	VAL	N-CA-C	-5.65	102.29	109.58
1	D	288	VAL	N-CA-C	-5.64	102.30	109.58
1	B	288	VAL	N-CA-C	-5.62	102.33	109.58
1	C	375	TYR	CA-C-N	-5.47	113.00	119.84
1	C	375	TYR	C-N-CA	-5.47	113.00	119.84
1	B	375	TYR	CA-C-N	-5.44	113.04	119.84
1	B	375	TYR	C-N-CA	-5.44	113.04	119.84
1	A	375	TYR	CA-C-N	-5.43	113.05	119.84
1	A	375	TYR	C-N-CA	-5.43	113.05	119.84
1	D	375	TYR	CA-C-N	-5.43	113.06	119.84
1	D	375	TYR	C-N-CA	-5.43	113.06	119.84
1	C	63	ILE	N-CA-C	-5.26	104.52	111.09
1	D	188	THR	N-CA-C	5.25	117.00	111.28
1	A	188	THR	N-CA-C	5.24	116.99	111.28
1	B	188	THR	N-CA-C	5.24	116.99	111.28
1	C	188	THR	N-CA-C	5.23	116.98	111.28
1	D	63	ILE	N-CA-C	-5.23	104.55	111.09
1	A	63	ILE	N-CA-C	-5.22	104.56	111.09
1	B	63	ILE	N-CA-C	-5.22	104.56	111.09
1	A	367	LYS	CA-C-N	-5.22	113.81	119.24
1	A	367	LYS	C-N-CA	-5.22	113.81	119.24
1	B	367	LYS	CA-C-N	-5.21	113.82	119.24
1	B	367	LYS	C-N-CA	-5.21	113.82	119.24
1	B	422	ALA	N-CA-C	5.21	112.82	108.13
1	C	367	LYS	CA-C-N	-5.21	113.82	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	LYS	C-N-CA	-5.21	113.82	119.24
1	A	422	ALA	N-CA-C	5.19	112.80	108.13
1	C	290	SER	N-CA-C	5.17	117.36	110.53
1	D	367	LYS	CA-C-N	-5.17	113.86	119.24
1	D	367	LYS	C-N-CA	-5.17	113.86	119.24
1	D	422	ALA	N-CA-C	5.17	112.78	108.13
1	A	290	SER	N-CA-C	5.16	117.34	110.53
1	B	290	SER	N-CA-C	5.15	117.32	110.53
1	C	422	ALA	N-CA-C	5.14	112.76	108.13
1	D	290	SER	N-CA-C	5.14	117.32	110.53
1	B	242	ASN	CA-C-N	5.12	125.16	119.32
1	B	242	ASN	C-N-CA	5.12	125.16	119.32
1	C	374	ILE	N-CA-C	-5.12	106.45	111.77
1	D	183	HIS	N-CA-C	-5.08	99.51	108.20
1	A	242	ASN	CA-C-N	5.08	125.11	119.32
1	A	242	ASN	C-N-CA	5.08	125.11	119.32
1	A	183	HIS	N-CA-C	-5.07	99.54	108.20
1	B	183	HIS	N-CA-C	-5.07	99.53	108.20
1	A	374	ILE	N-CA-C	-5.06	106.50	111.77
1	B	374	ILE	N-CA-C	-5.06	106.50	111.77
1	C	183	HIS	N-CA-C	-5.06	99.54	108.20
1	C	242	ASN	CA-C-N	5.06	125.09	119.32
1	C	242	ASN	C-N-CA	5.06	125.09	119.32
1	D	242	ASN	CA-C-N	5.06	125.09	119.32
1	D	242	ASN	C-N-CA	5.06	125.09	119.32
1	D	12	VAL	N-CA-C	5.04	115.84	108.53
1	A	12	VAL	N-CA-C	5.04	115.84	108.53
1	B	12	VAL	N-CA-C	5.03	115.83	108.53
1	D	374	ILE	N-CA-C	-5.03	106.54	111.77
1	C	12	VAL	N-CA-C	5.02	115.81	108.53
1	B	276	GLU	N-CA-C	5.00	116.73	111.28
1	C	276	GLU	N-CA-C	5.00	116.73	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3420	0	3410	144	2
1	B	3420	0	3410	156	5
1	C	3420	0	3410	149	2
1	D	3420	0	3410	153	5
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	124	0	0	5	0
3	B	129	0	0	6	1
3	C	128	0	0	8	0
3	D	127	0	0	7	1
All	All	14196	0	13640	570	8

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 21.

All (570) 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:164:GLY:H	1:D:188:THR:CG2	1.35	1.38
1:D:71:ARG:HD3	3:D:2016:HOH:O	1.24	1.32
1:C:71:ARG:HD3	3:C:2016:HOH:O	1.28	1.29
1:C:70:ASN:HA	3:C:2014:HOH:O	1.46	1.15
1:A:188:THR:CG2	1:C:164:GLY:H	1.61	1.13
1:B:164:GLY:N	1:D:188:THR:CG2	2.09	1.13
1:A:164:GLY:H	1:C:188:THR:CG2	1.61	1.12
1:B:164:GLY:H	1:D:188:THR:HG21	1.15	1.04
1:B:188:THR:CG2	1:D:164:GLY:H	1.70	1.03
1:C:266:GLN:H	1:C:266:GLN:HE21	1.08	0.99
1:A:266:GLN:H	1:A:266:GLN:HE21	1.08	0.97
1:B:7:LYS:NZ	3:B:2003:HOH:O	1.99	0.94
1:D:266:GLN:H	1:D:266:GLN:HE21	1.08	0.93
1:B:266:GLN:HE21	1:B:266:GLN:H	1.08	0.93
1:A:271:THR:HG22	1:A:273:ASP:H	1.35	0.90
1:B:271:THR:HG22	1:B:273:ASP:H	1.36	0.90
1:C:271:THR:HG22	1:C:273:ASP:H	1.36	0.90
1:D:408:LEU:HD11	3:D:2014:HOH:O	1.71	0.90
1:D:271:THR:HG22	1:D:273:ASP:H	1.36	0.89
1:B:243:PRO:HD2	1:B:293:MET:HE2	1.55	0.88
1:C:243:PRO:HD2	1:C:293:MET:HE2	1.55	0.88
1:D:243:PRO:HD2	1:D:293:MET:HE2	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLY:N	1:D:188:THR:HG22	1.87	0.88
1:A:243:PRO:HD2	1:A:293:MET:HE2	1.55	0.88
1:B:266:GLN:H	1:B:266:GLN:NE2	1.71	0.88
1:D:266:GLN:H	1:D:266:GLN:NE2	1.71	0.88
1:C:266:GLN:H	1:C:266:GLN:NE2	1.71	0.86
1:A:266:GLN:H	1:A:266:GLN:NE2	1.71	0.86
1:A:164:GLY:N	1:C:188:THR:CG2	2.41	0.84
1:B:188:THR:HG21	1:D:164:GLY:H	1.39	0.84
1:B:4:VAL:HG13	1:B:24:VAL:HG13	1.60	0.83
1:A:4:VAL:HG13	1:A:24:VAL:HG13	1.61	0.83
1:A:188:THR:CG2	1:C:164:GLY:N	2.41	0.83
1:C:4:VAL:HG13	1:C:24:VAL:HG13	1.60	0.82
1:A:342:LEU:HD22	1:A:346:LEU:HD22	1.61	0.82
1:B:342:LEU:HD22	1:B:346:LEU:HD22	1.61	0.82
1:D:4:VAL:HG13	1:D:24:VAL:HG13	1.60	0.82
1:D:342:LEU:HD22	1:D:346:LEU:HD22	1.61	0.81
1:C:342:LEU:HD22	1:C:346:LEU:HD22	1.61	0.81
1:A:31:ALA:HB2	1:B:33:SER:HB2	1.63	0.80
1:B:188:THR:CG2	1:D:164:GLY:N	2.45	0.79
1:C:71:ARG:CD	3:C:2016:HOH:O	2.02	0.79
1:C:450:THR:O	1:C:451:ARG:HB3	1.82	0.79
1:B:102:THR:HG22	1:B:104:ASP:H	1.49	0.78
1:D:450:THR:O	1:D:451:ARG:HB3	1.82	0.78
1:D:102:THR:HG22	1:D:104:ASP:H	1.49	0.78
1:B:450:THR:O	1:B:451:ARG:HB3	1.82	0.77
1:C:102:THR:HG22	1:C:104:ASP:H	1.49	0.77
1:A:102:THR:HG22	1:A:104:ASP:H	1.49	0.77
1:D:264:GLY:HA3	1:D:266:GLN:HE22	1.50	0.77
1:A:450:THR:O	1:A:451:ARG:HB3	1.82	0.77
1:B:264:GLY:HA3	1:B:266:GLN:HE22	1.50	0.76
1:A:188:THR:HG21	1:C:164:GLY:H	1.50	0.75
1:C:264:GLY:HA3	1:C:266:GLN:HE22	1.50	0.75
1:A:264:GLY:HA3	1:A:266:GLN:HE22	1.50	0.74
1:D:76:GLU:HG3	1:D:116:ARG:HB3	1.70	0.74
1:A:76:GLU:HG3	1:A:116:ARG:HB3	1.70	0.74
1:C:278:ILE:HB	1:C:282:MET:CE	2.18	0.73
1:C:76:GLU:HG3	1:C:116:ARG:HB3	1.70	0.73
1:B:278:ILE:HB	1:B:282:MET:CE	2.18	0.73
1:A:164:GLY:H	1:C:188:THR:HG22	1.51	0.73
1:A:164:GLY:H	1:C:188:THR:HG21	1.50	0.73
1:B:76:GLU:HG3	1:B:116:ARG:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HB	1:A:282:MET:CE	2.18	0.72
1:D:278:ILE:HB	1:D:282:MET:CE	2.18	0.72
1:B:164:GLY:H	1:D:188:THR:HG23	1.50	0.72
1:B:375:TYR:O	1:B:376:PRO:C	2.31	0.72
1:C:344:MET:HE3	1:C:348:ASN:HD21	1.55	0.71
1:A:33:SER:HB2	1:B:31:ALA:HB2	1.71	0.71
1:A:375:TYR:O	1:A:376:PRO:C	2.31	0.71
1:C:375:TYR:O	1:C:376:PRO:C	2.31	0.70
1:A:188:THR:HG22	1:C:164:GLY:H	1.51	0.70
1:B:344:MET:HE3	1:B:348:ASN:HD21	1.56	0.70
1:D:344:MET:HE3	1:D:348:ASN:HD21	1.55	0.70
1:A:344:MET:HE3	1:A:348:ASN:HD21	1.56	0.70
1:D:375:TYR:O	1:D:376:PRO:C	2.31	0.69
1:A:164:GLY:N	1:C:188:THR:HG22	2.07	0.69
1:D:451:ARG:HG3	1:D:451:ARG:HH11	1.58	0.69
1:A:188:THR:HG22	1:C:164:GLY:N	2.07	0.69
1:D:12:VAL:HG22	1:D:361:VAL:HG21	1.75	0.68
1:A:271:THR:HG22	1:A:273:ASP:N	2.09	0.68
1:B:12:VAL:HG22	1:B:361:VAL:HG21	1.75	0.68
1:A:102:THR:HG22	1:A:104:ASP:N	2.09	0.68
1:A:451:ARG:HG3	1:A:451:ARG:HH11	1.58	0.68
1:A:5:ILE:HG12	1:A:23:LEU:HD13	1.76	0.68
1:B:271:THR:HG22	1:B:273:ASP:N	2.09	0.67
1:C:451:ARG:HG3	1:C:451:ARG:HH11	1.58	0.67
1:A:12:VAL:HG22	1:A:361:VAL:HG21	1.75	0.67
1:C:102:THR:HG22	1:C:104:ASP:N	2.09	0.67
1:B:102:THR:HG22	1:B:104:ASP:N	2.09	0.67
1:D:271:THR:HG22	1:D:273:ASP:N	2.09	0.67
1:B:5:ILE:HG12	1:B:23:LEU:HD13	1.76	0.67
1:D:5:ILE:HG12	1:D:23:LEU:HD13	1.76	0.67
1:B:451:ARG:HG3	1:B:451:ARG:HH11	1.58	0.67
1:C:5:ILE:HG12	1:C:23:LEU:HD13	1.76	0.67
1:D:102:THR:HG22	1:D:104:ASP:N	2.09	0.66
1:C:12:VAL:HG22	1:C:361:VAL:HG21	1.75	0.66
1:C:271:THR:HG22	1:C:273:ASP:N	2.09	0.66
1:B:426:THR:HG23	1:B:434:ALA:HB3	1.79	0.65
1:D:426:THR:HG23	1:D:434:ALA:HB3	1.79	0.65
1:B:296:ARG:HG3	1:B:296:ARG:HH11	1.62	0.64
1:A:426:THR:HG23	1:A:434:ALA:HB3	1.79	0.64
1:A:162:SER:OG	1:A:165:GLU:HG3	1.98	0.64
1:B:162:SER:OG	1:B:165:GLU:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ALA:HB2	1:D:33:SER:HB2	1.80	0.64
1:C:426:THR:HG23	1:C:434:ALA:HB3	1.79	0.63
1:D:296:ARG:HG3	1:D:296:ARG:HH11	1.62	0.63
1:C:162:SER:OG	1:C:165:GLU:HG3	1.98	0.63
1:D:162:SER:OG	1:D:165:GLU:HG3	1.98	0.63
1:C:296:ARG:HG3	1:C:296:ARG:HH11	1.62	0.63
1:A:296:ARG:HG3	1:A:296:ARG:HH11	1.62	0.63
1:B:281:TYR:O	1:B:413:PRO:HG3	1.99	0.63
1:C:10:ARG:HG2	1:C:17:ILE:HG21	1.81	0.63
1:C:281:TYR:O	1:C:413:PRO:HG3	1.99	0.62
1:A:281:TYR:O	1:A:413:PRO:HG3	1.99	0.62
1:C:204:ASP:HB2	1:C:207:ALA:H	1.65	0.62
1:A:10:ARG:HG2	1:A:17:ILE:HG21	1.81	0.62
1:B:204:ASP:HB2	1:B:207:ALA:H	1.65	0.62
1:B:373:GLY:O	1:B:451:ARG:HG2	1.99	0.62
1:D:69:LYS:HB2	1:D:74:ARG:HD2	1.82	0.62
1:C:69:LYS:HB2	1:C:74:ARG:HD2	1.82	0.62
1:B:10:ARG:HG2	1:B:17:ILE:HG21	1.81	0.61
1:A:373:GLY:O	1:A:451:ARG:HG2	1.99	0.61
1:B:188:THR:HG22	1:D:164:GLY:N	2.16	0.61
1:D:373:GLY:O	1:D:451:ARG:HG2	1.99	0.61
1:C:373:GLY:O	1:C:451:ARG:HG2	1.99	0.61
1:D:83:ALA:O	1:D:426:THR:HG21	2.00	0.61
1:D:281:TYR:O	1:D:413:PRO:HG3	1.99	0.61
1:D:10:ARG:HG2	1:D:17:ILE:HG21	1.82	0.61
1:A:69:LYS:HB2	1:A:74:ARG:HD2	1.82	0.61
1:B:83:ALA:O	1:B:426:THR:HG21	2.00	0.61
1:C:83:ALA:O	1:C:426:THR:HG21	2.00	0.61
1:A:83:ALA:O	1:A:426:THR:HG21	2.00	0.61
1:B:69:LYS:HB2	1:B:74:ARG:HD2	1.82	0.61
1:C:33:SER:HB2	1:D:31:ALA:HB2	1.83	0.60
1:A:4:VAL:HG13	1:A:24:VAL:CG1	2.30	0.60
1:A:204:ASP:HB2	1:A:207:ALA:H	1.65	0.60
1:B:36:THR:O	1:B:39:VAL:HG22	2.01	0.60
1:B:164:GLY:CA	1:D:188:THR:CG2	2.79	0.60
1:B:340:THR:O	1:B:344:MET:HB2	2.02	0.60
1:D:340:THR:O	1:D:344:MET:HB2	2.02	0.60
1:A:340:THR:O	1:A:344:MET:HB2	2.02	0.60
1:D:204:ASP:HB2	1:D:207:ALA:H	1.65	0.60
1:A:128:VAL:HB	1:A:129:PRO:HD2	1.84	0.59
1:D:128:VAL:HB	1:D:129:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:VAL:HG13	1:D:24:VAL:CG1	2.30	0.59
1:A:275:ALA:HA	1:A:282:MET:HE1	1.85	0.59
1:A:36:THR:O	1:A:39:VAL:HG22	2.01	0.59
1:B:275:ALA:HA	1:B:282:MET:HE1	1.85	0.59
1:C:36:THR:O	1:C:39:VAL:HG22	2.01	0.59
1:D:36:THR:O	1:D:39:VAL:HG22	2.01	0.59
1:B:128:VAL:HB	1:B:129:PRO:HD2	1.84	0.59
1:D:275:ALA:HA	1:D:282:MET:HE1	1.85	0.59
1:C:340:THR:O	1:C:344:MET:HB2	2.02	0.59
1:B:4:VAL:HG13	1:B:24:VAL:CG1	2.30	0.58
1:C:4:VAL:HG13	1:C:24:VAL:CG1	2.30	0.58
1:B:80:GLU:HG2	1:B:118:LYS:HD2	1.86	0.58
1:D:62:HIS:CE1	1:D:93:MET:HG3	2.39	0.58
1:A:62:HIS:CE1	1:A:93:MET:HG3	2.39	0.58
1:C:128:VAL:HB	1:C:129:PRO:HD2	1.84	0.58
1:B:164:GLY:HA3	1:D:188:THR:HG23	1.84	0.58
1:C:10:ARG:HG2	1:C:17:ILE:CG2	2.34	0.57
1:D:80:GLU:HG2	1:D:118:LYS:HD2	1.86	0.57
1:B:10:ARG:HG2	1:B:17:ILE:CG2	2.34	0.57
1:A:10:ARG:HG2	1:A:17:ILE:CG2	2.34	0.57
1:A:80:GLU:HG2	1:A:118:LYS:HD2	1.86	0.57
1:B:62:HIS:CE1	1:B:93:MET:HG3	2.39	0.57
1:C:275:ALA:HA	1:C:282:MET:HE1	1.85	0.57
1:C:62:HIS:CE1	1:C:93:MET:HG3	2.39	0.56
1:C:80:GLU:HG2	1:C:118:LYS:HD2	1.86	0.56
1:C:212:GLN:O	1:C:289:ARG:NH2	2.38	0.56
1:D:10:ARG:HG2	1:D:17:ILE:CG2	2.34	0.56
1:A:375:TYR:O	1:A:377:GLN:N	2.38	0.56
1:B:212:GLN:O	1:B:289:ARG:NH2	2.38	0.56
1:A:274:ASP:C	1:A:282:MET:HE1	2.31	0.56
1:B:164:GLY:CA	1:D:188:THR:HG23	2.36	0.56
1:D:375:TYR:O	1:D:377:GLN:N	2.38	0.56
1:B:100:THR:OG1	1:B:109:LYS:HE3	2.06	0.56
1:B:375:TYR:O	1:B:377:GLN:N	2.38	0.56
1:D:274:ASP:C	1:D:282:MET:HE1	2.31	0.56
1:D:188:THR:HB	3:D:2051:HOH:O	2.06	0.56
1:A:100:THR:OG1	1:A:109:LYS:HE3	2.06	0.56
1:A:212:GLN:O	1:A:289:ARG:NH2	2.38	0.56
1:B:188:THR:HB	3:B:2050:HOH:O	2.06	0.56
1:C:274:ASP:C	1:C:282:MET:HE1	2.31	0.56
1:C:375:TYR:O	1:C:377:GLN:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLY:N	1:D:188:THR:HG23	2.12	0.55
1:A:149:MET:HE2	1:A:158:PHE:CD2	2.42	0.55
1:B:274:ASP:C	1:B:282:MET:HE1	2.31	0.55
1:C:210:ALA:O	1:C:213:PRO:HD3	2.07	0.55
1:D:149:MET:HE2	1:D:158:PHE:CD2	2.42	0.55
1:A:210:ALA:O	1:A:213:PRO:HD3	2.07	0.55
1:B:89:THR:HG21	1:B:378:LYS:HD2	1.89	0.55
1:B:149:MET:HE2	1:B:158:PHE:CD2	2.42	0.55
1:C:100:THR:OG1	1:C:109:LYS:HE3	2.06	0.55
1:D:210:ALA:O	1:D:213:PRO:HD3	2.07	0.55
1:A:93:MET:HE3	1:A:124:TYR:CD2	2.42	0.55
1:A:188:THR:HB	3:A:2047:HOH:O	2.06	0.55
1:C:188:THR:HB	3:C:2051:HOH:O	2.06	0.54
1:D:89:THR:HG21	1:D:378:LYS:HD2	1.89	0.54
1:B:154:VAL:HG23	1:B:154:VAL:O	2.08	0.54
1:C:149:MET:HE2	1:C:158:PHE:CD2	2.42	0.54
1:D:100:THR:OG1	1:D:109:LYS:HE3	2.06	0.54
1:B:93:MET:HE3	1:B:124:TYR:CD2	2.42	0.54
1:C:93:MET:HE3	1:C:124:TYR:CD2	2.42	0.54
1:D:212:GLN:O	1:D:289:ARG:NH2	2.38	0.54
1:D:278:ILE:HB	1:D:282:MET:HE3	1.90	0.54
1:A:278:ILE:HB	1:A:282:MET:HE3	1.90	0.54
1:A:451:ARG:HG3	1:A:451:ARG:NH1	2.22	0.54
1:B:210:ALA:O	1:B:213:PRO:HD3	2.07	0.54
1:C:451:ARG:HG3	1:C:451:ARG:NH1	2.22	0.54
1:A:89:THR:HG21	1:A:378:LYS:HD2	1.89	0.54
1:C:154:VAL:O	1:C:154:VAL:HG23	2.08	0.54
1:D:93:MET:HE3	1:D:124:TYR:CD2	2.42	0.54
1:A:435:GLU:HG2	1:A:436:LYS:HG2	1.91	0.53
1:C:278:ILE:HB	1:C:282:MET:HE3	1.90	0.53
1:D:136:ARG:HB2	3:D:2034:HOH:O	2.09	0.53
1:D:154:VAL:HG23	1:D:154:VAL:O	2.08	0.53
1:B:278:ILE:HB	1:B:282:MET:HE3	1.90	0.53
1:C:89:THR:HG21	1:C:378:LYS:HD2	1.89	0.53
1:C:136:ARG:HB2	3:C:2034:HOH:O	2.09	0.53
1:A:396:ILE:HG22	1:A:397:ASP:N	2.23	0.53
1:C:396:ILE:HG22	1:C:397:ASP:N	2.23	0.53
1:D:204:ASP:CB	1:D:207:ALA:H	2.21	0.53
1:A:154:VAL:HG23	1:A:154:VAL:O	2.08	0.53
1:B:136:ARG:HB2	3:B:2033:HOH:O	2.09	0.53
1:D:296:ARG:HG3	1:D:296:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HG3	1:A:296:ARG:NH1	2.24	0.53
1:D:282:MET:O	1:D:282:MET:HG2	2.08	0.53
1:D:396:ILE:HG22	1:D:397:ASP:N	2.23	0.53
1:B:282:MET:O	1:B:282:MET:HG2	2.08	0.53
1:C:204:ASP:CB	1:C:207:ALA:H	2.21	0.53
1:A:204:ASP:CB	1:A:207:ALA:H	2.21	0.53
1:C:282:MET:O	1:C:282:MET:HG2	2.08	0.53
1:C:435:GLU:HG2	1:C:436:LYS:HG2	1.91	0.53
1:B:396:ILE:HG22	1:B:397:ASP:N	2.23	0.53
1:B:435:GLU:HG2	1:B:436:LYS:HG2	1.91	0.53
1:C:296:ARG:HG3	1:C:296:ARG:NH1	2.24	0.53
1:A:93:MET:HE1	1:A:147:KCX:HB3	1.91	0.52
1:B:164:GLY:N	1:D:188:THR:HG21	1.97	0.52
1:D:435:GLU:HG2	1:D:436:LYS:HG2	1.91	0.52
1:C:301:LEU:O	1:C:359:ARG:HD3	2.09	0.52
1:A:282:MET:HG2	1:A:282:MET:O	2.08	0.52
1:D:301:LEU:O	1:D:359:ARG:HD3	2.09	0.52
1:B:301:LEU:O	1:B:359:ARG:HD3	2.09	0.52
1:D:93:MET:HE1	1:D:147:KCX:HB3	1.91	0.52
1:A:136:ARG:HB2	3:A:2031:HOH:O	2.09	0.52
1:B:204:ASP:CB	1:B:207:ALA:H	2.21	0.52
1:B:10:ARG:HD2	1:B:51:PHE:CE1	2.45	0.52
1:B:93:MET:HE1	1:B:147:KCX:HB3	1.91	0.52
1:C:147:KCX:HG3	1:C:148:SER:N	2.25	0.52
1:A:301:LEU:O	1:A:359:ARG:HD3	2.09	0.52
1:B:147:KCX:HG3	1:B:148:SER:N	2.25	0.51
1:A:10:ARG:HD2	1:A:51:PHE:CE1	2.45	0.51
1:A:147:KCX:HG3	1:A:148:SER:N	2.25	0.51
1:C:93:MET:HE1	1:C:147:KCX:HB3	1.91	0.51
1:D:147:KCX:HG3	1:D:148:SER:N	2.25	0.51
1:A:375:TYR:HB3	1:A:376:PRO:CD	2.41	0.51
1:C:10:ARG:HD2	1:C:51:PHE:CE1	2.45	0.51
1:A:400:VAL:HG12	1:A:417:MET:O	2.11	0.51
1:B:296:ARG:HG3	1:B:296:ARG:NH1	2.24	0.51
1:B:400:VAL:CG1	1:B:414:PHE:O	2.59	0.51
1:D:400:VAL:HG12	1:D:417:MET:O	2.11	0.51
1:A:344:MET:HE3	1:A:348:ASN:ND2	2.25	0.50
1:A:400:VAL:CG1	1:A:414:PHE:O	2.59	0.50
1:C:375:TYR:HB3	1:C:376:PRO:CD	2.41	0.50
1:D:375:TYR:HB3	1:D:376:PRO:CD	2.41	0.50
1:B:302:GLU:OE1	1:B:355:LEU:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:VAL:HG12	1:B:417:MET:O	2.11	0.50
1:C:302:GLU:OE1	1:C:355:LEU:HA	2.12	0.50
1:B:71:ARG:CZ	1:B:71:ARG:HB2	2.41	0.50
1:A:2:PHE:O	1:A:41:ALA:HA	2.12	0.50
1:A:71:ARG:HB2	1:A:71:ARG:CZ	2.41	0.50
1:A:266:GLN:HE21	1:A:266:GLN:N	1.92	0.50
1:B:204:ASP:HB3	1:B:206:ALA:H	1.77	0.50
1:D:204:ASP:HB3	1:D:206:ALA:H	1.76	0.50
1:B:344:MET:HE3	1:B:348:ASN:ND2	2.25	0.50
1:D:10:ARG:HD2	1:D:51:PHE:CE1	2.45	0.50
1:D:451:ARG:HG3	1:D:451:ARG:NH1	2.22	0.50
1:D:71:ARG:HB2	1:D:71:ARG:CZ	2.41	0.50
1:B:23:LEU:HD22	1:B:23:LEU:N	2.27	0.50
1:B:375:TYR:HB3	1:B:376:PRO:CD	2.41	0.50
1:C:400:VAL:HG12	1:C:417:MET:O	2.11	0.50
1:A:63:ILE:N	1:A:92:GLU:OE2	2.34	0.50
1:C:23:LEU:N	1:C:23:LEU:HD22	2.27	0.50
1:A:204:ASP:HB3	1:A:206:ALA:H	1.77	0.49
1:C:71:ARG:HB2	1:C:71:ARG:CZ	2.41	0.49
1:D:23:LEU:N	1:D:23:LEU:HD22	2.27	0.49
1:C:400:VAL:CG1	1:C:414:PHE:O	2.59	0.49
1:D:181:VAL:HG12	1:D:236:ILE:HB	1.94	0.49
1:D:375:TYR:CG	1:D:376:PRO:N	2.79	0.49
1:A:23:LEU:N	1:A:23:LEU:HD22	2.27	0.49
1:C:181:VAL:HG12	1:C:236:ILE:HB	1.94	0.49
1:D:2:PHE:O	1:D:41:ALA:HA	2.12	0.49
1:C:2:PHE:O	1:C:41:ALA:HA	2.12	0.49
1:C:204:ASP:HB3	1:C:206:ALA:H	1.77	0.49
1:C:344:MET:HE3	1:C:348:ASN:ND2	2.25	0.49
1:D:271:THR:CG2	1:D:273:ASP:H	2.18	0.49
1:D:302:GLU:OE1	1:D:355:LEU:HA	2.12	0.49
1:D:400:VAL:CG1	1:D:414:PHE:O	2.59	0.49
1:A:302:GLU:OE1	1:A:355:LEU:HA	2.12	0.49
1:B:264:GLY:CA	1:B:266:GLN:HE22	2.24	0.49
1:C:161:VAL:HB	1:C:165:GLU:HB2	1.94	0.49
1:D:161:VAL:HB	1:D:165:GLU:HB2	1.94	0.49
1:D:23:LEU:N	1:D:23:LEU:CD2	2.76	0.49
1:A:271:THR:CG2	1:A:273:ASP:H	2.18	0.49
1:C:23:LEU:N	1:C:23:LEU:CD2	2.76	0.49
1:B:2:PHE:O	1:B:41:ALA:HA	2.12	0.49
1:A:181:VAL:HG12	1:A:236:ILE:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ILE:N	1:D:17:ILE:HD12	2.28	0.49
1:D:344:MET:HE3	1:D:348:ASN:ND2	2.25	0.49
1:A:161:VAL:HB	1:A:165:GLU:HB2	1.94	0.48
1:B:17:ILE:N	1:B:17:ILE:HD12	2.28	0.48
1:B:23:LEU:N	1:B:23:LEU:CD2	2.76	0.48
1:B:181:VAL:HG12	1:B:236:ILE:HB	1.94	0.48
1:C:292:GLU:HG3	3:C:2086:HOH:O	2.13	0.48
1:B:161:VAL:HB	1:B:165:GLU:HB2	1.94	0.48
1:B:264:GLY:C	1:B:266:GLN:NE2	2.72	0.48
1:D:292:GLU:HG3	3:D:2085:HOH:O	2.13	0.48
1:A:17:ILE:N	1:A:17:ILE:HD12	2.28	0.48
1:A:23:LEU:N	1:A:23:LEU:CD2	2.76	0.48
1:C:271:THR:CG2	1:C:272:THR:N	2.77	0.48
1:C:17:ILE:HD12	1:C:17:ILE:N	2.28	0.48
1:D:266:GLN:HE21	1:D:266:GLN:N	1.92	0.48
1:B:230:GLU:HG2	1:D:215:PHE:CE2	2.48	0.48
1:B:292:GLU:HG3	3:B:2085:HOH:O	2.13	0.48
1:A:264:GLY:CA	1:A:266:GLN:HE22	2.24	0.48
1:A:292:GLU:HG3	3:A:2082:HOH:O	2.13	0.48
1:B:97:PHE:HA	1:B:98:PRO:C	2.39	0.48
1:B:451:ARG:HG3	1:B:451:ARG:NH1	2.22	0.48
1:A:97:PHE:HA	1:A:98:PRO:C	2.39	0.47
1:A:264:GLY:C	1:A:266:GLN:NE2	2.72	0.47
1:B:271:THR:CG2	1:B:272:THR:N	2.77	0.47
1:C:218:ASN:HD21	1:C:242:ASN:HD21	1.63	0.47
1:C:322:GLU:N	1:C:323:PRO:HD2	2.29	0.47
1:D:54:PRO:HG3	1:D:381:LEU:HD22	1.96	0.47
1:D:97:PHE:HA	1:D:98:PRO:C	2.39	0.47
1:D:218:ASN:HD21	1:D:242:ASN:HD21	1.62	0.47
1:C:222:GLN:HE21	1:C:222:GLN:HB2	1.50	0.47
1:D:264:GLY:C	1:D:266:GLN:NE2	2.72	0.47
1:A:54:PRO:HG3	1:A:381:LEU:HD22	1.96	0.47
1:A:375:TYR:CG	1:A:376:PRO:N	2.79	0.47
1:B:241:SER:OG	1:B:289:ARG:HD3	2.14	0.47
1:C:241:SER:OG	1:C:289:ARG:HD3	2.14	0.47
1:A:271:THR:CG2	1:A:272:THR:N	2.77	0.47
1:A:283:LYS:HE2	1:A:333:ASN:OD1	2.15	0.47
1:B:93:MET:HE3	1:B:93:MET:HA	1.97	0.47
1:C:97:PHE:HA	1:C:98:PRO:C	2.39	0.47
1:C:264:GLY:C	1:C:266:GLN:NE2	2.72	0.47
1:D:283:LYS:HE2	1:D:333:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:N	1:A:323:PRO:HD2	2.29	0.47
1:B:322:GLU:N	1:B:323:PRO:HD2	2.29	0.47
1:D:322:GLU:N	1:D:323:PRO:HD2	2.29	0.47
1:A:241:SER:OG	1:A:289:ARG:HD3	2.14	0.47
1:C:54:PRO:HG3	1:C:381:LEU:HD22	1.96	0.47
1:B:218:ASN:HD21	1:B:242:ASN:HD21	1.62	0.47
1:C:283:LYS:HE2	1:C:333:ASN:OD1	2.15	0.47
1:C:375:TYR:CG	1:C:376:PRO:N	2.79	0.47
1:D:271:THR:CG2	1:D:272:THR:N	2.77	0.47
1:D:375:TYR:O	1:D:378:LYS:O	2.33	0.47
1:A:375:TYR:O	1:A:378:LYS:O	2.33	0.47
1:B:375:TYR:O	1:B:378:LYS:O	2.33	0.47
1:C:266:GLN:HE21	1:C:266:GLN:N	1.92	0.47
1:C:173:ILE:HG13	1:C:180:ILE:HB	1.98	0.46
1:C:375:TYR:O	1:C:378:LYS:O	2.33	0.46
1:A:204:ASP:HB3	1:A:206:ALA:N	2.30	0.46
1:C:405:PHE:O	1:C:410:LYS:HE3	2.16	0.46
1:D:241:SER:OG	1:D:289:ARG:HD3	2.14	0.46
1:B:277:ARG:HH22	1:B:417:MET:HE2	1.81	0.46
1:C:277:ARG:HH22	1:C:417:MET:HE2	1.81	0.46
1:B:54:PRO:HG3	1:B:381:LEU:HD22	1.96	0.46
1:B:226:LEU:HD23	1:D:219:GLU:HA	1.96	0.46
1:C:204:ASP:HB3	1:C:206:ALA:N	2.30	0.46
1:D:204:ASP:HB3	1:D:206:ALA:N	2.30	0.46
1:B:283:LYS:HE2	1:B:333:ASN:OD1	2.15	0.46
1:A:93:MET:HE3	1:A:93:MET:HA	1.97	0.46
1:A:173:ILE:HG13	1:A:180:ILE:HB	1.98	0.46
1:A:277:ARG:HH22	1:A:417:MET:HE2	1.81	0.46
1:D:405:PHE:O	1:D:410:LYS:HE3	2.15	0.46
1:B:102:THR:CG2	1:B:103:LEU:N	2.79	0.46
1:D:338:LEU:HD12	1:D:338:LEU:HA	1.83	0.46
1:A:405:PHE:O	1:A:410:LYS:HE3	2.15	0.45
1:D:305:LEU:HD12	1:D:305:LEU:N	2.31	0.45
1:B:173:ILE:HG13	1:B:180:ILE:HB	1.98	0.45
1:B:405:PHE:O	1:B:410:LYS:HE3	2.16	0.45
1:D:228:GLN:HG2	1:D:259:VAL:CG1	2.46	0.45
1:B:204:ASP:HB3	1:B:206:ALA:N	2.30	0.45
1:B:342:LEU:HB3	1:B:343:PRO:CD	2.47	0.45
1:B:375:TYR:CG	1:B:376:PRO:N	2.79	0.45
1:C:93:MET:HE3	1:C:93:MET:HA	1.97	0.45
1:C:305:LEU:N	1:C:305:LEU:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ARG:HG3	1:C:234:ARG:HH11	1.82	0.45
1:C:271:THR:CG2	1:C:273:ASP:H	2.18	0.45
1:A:228:GLN:HG2	1:A:259:VAL:CG1	2.46	0.45
1:A:342:LEU:HB3	1:A:343:PRO:CD	2.47	0.45
1:B:228:GLN:HG2	1:B:259:VAL:CG1	2.46	0.45
1:D:264:GLY:CA	1:D:266:GLN:HE22	2.24	0.45
1:A:31:ALA:CB	1:B:33:SER:HB2	2.38	0.45
1:C:342:LEU:HB3	1:C:343:PRO:CD	2.47	0.45
1:D:93:MET:HE3	1:D:93:MET:HA	1.97	0.45
1:D:296:ARG:O	1:D:300:GLN:HG3	2.17	0.45
1:A:271:THR:HB	3:A:2076:HOH:O	2.16	0.45
1:B:305:LEU:N	1:B:305:LEU:HD12	2.31	0.45
1:D:342:LEU:HB3	1:D:343:PRO:CD	2.47	0.45
1:A:218:ASN:HD21	1:A:242:ASN:HD21	1.62	0.45
1:B:63:ILE:N	1:B:92:GLU:OE2	2.34	0.45
1:B:149:MET:HE2	1:B:158:PHE:HD2	1.82	0.45
1:C:264:GLY:CA	1:C:266:GLN:HE22	2.24	0.45
1:D:390:LEU:HD22	1:D:426:THR:HB	1.99	0.45
1:A:296:ARG:O	1:A:300:GLN:HG3	2.17	0.44
1:A:390:LEU:CD2	1:A:426:THR:HB	2.47	0.44
1:B:266:GLN:HE21	1:B:266:GLN:N	1.92	0.44
1:B:271:THR:HB	3:B:2079:HOH:O	2.16	0.44
1:B:390:LEU:CD2	1:B:426:THR:HB	2.47	0.44
1:C:296:ARG:O	1:C:300:GLN:HG3	2.17	0.44
1:C:390:LEU:HD22	1:C:426:THR:HB	1.99	0.44
1:D:173:ILE:HG13	1:D:180:ILE:HB	1.98	0.44
1:C:228:GLN:HG2	1:C:259:VAL:CG1	2.46	0.44
1:C:390:LEU:CD2	1:C:426:THR:HB	2.47	0.44
1:D:149:MET:HE2	1:D:158:PHE:HD2	1.82	0.44
1:D:390:LEU:CD2	1:D:426:THR:HB	2.47	0.44
1:A:102:THR:CG2	1:A:103:LEU:N	2.79	0.44
1:A:234:ARG:HG3	1:A:234:ARG:HH11	1.82	0.44
1:A:400:VAL:HG11	1:A:414:PHE:O	2.18	0.44
1:D:396:ILE:CG2	1:D:397:ASP:N	2.81	0.44
1:D:434:ALA:HA	1:D:438:GLU:O	2.17	0.44
1:A:305:LEU:HD12	1:A:305:LEU:N	2.31	0.44
1:B:400:VAL:HG11	1:B:414:PHE:O	2.18	0.44
1:C:400:VAL:HG11	1:C:414:PHE:O	2.18	0.44
1:C:434:ALA:HA	1:C:438:GLU:O	2.18	0.44
1:D:234:ARG:HH11	1:D:234:ARG:HG3	1.82	0.44
1:D:271:THR:HB	3:D:2079:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ILE:CG2	1:A:397:ASP:N	2.81	0.44
1:B:278:ILE:HB	1:B:282:MET:HE2	2.00	0.44
1:B:296:ARG:O	1:B:300:GLN:HG3	2.17	0.44
1:B:390:LEU:HD22	1:B:426:THR:HB	1.99	0.44
1:C:102:THR:CG2	1:C:103:LEU:N	2.79	0.44
1:C:271:THR:HB	3:C:2080:HOH:O	2.16	0.44
1:A:434:ALA:HA	1:A:438:GLU:O	2.17	0.44
1:C:63:ILE:N	1:C:92:GLU:OE2	2.34	0.44
1:C:313:HIS:CD2	1:C:338:LEU:HD22	2.53	0.43
1:C:396:ILE:CG2	1:C:397:ASP:N	2.81	0.43
1:A:285:ALA:HA	1:A:286:PRO:C	2.42	0.43
1:B:285:ALA:HA	1:B:286:PRO:C	2.42	0.43
1:B:234:ARG:HG3	1:B:234:ARG:HH11	1.82	0.43
1:D:400:VAL:HG11	1:D:414:PHE:O	2.18	0.43
1:A:55:GLY:HA3	1:A:88:THR:OG1	2.19	0.43
1:C:243:PRO:HD3	1:C:293:MET:HB3	2.00	0.43
1:D:313:HIS:CD2	1:D:338:LEU:HD22	2.54	0.43
1:A:243:PRO:HD3	1:A:293:MET:HB3	2.00	0.43
1:A:398:THR:HG23	1:A:419:VAL:HB	2.01	0.43
1:D:277:ARG:HH22	1:D:417:MET:HE2	1.81	0.43
1:A:390:LEU:HD22	1:A:426:THR:HB	1.99	0.43
1:C:55:GLY:HA3	1:C:88:THR:OG1	2.19	0.43
1:C:285:ALA:HA	1:C:286:PRO:C	2.43	0.43
1:D:102:THR:CG2	1:D:103:LEU:N	2.79	0.43
1:D:278:ILE:HB	1:D:282:MET:HE2	2.00	0.43
1:A:129:PRO:HB3	1:A:165:GLU:OE1	2.19	0.43
1:A:313:HIS:CD2	1:A:338:LEU:HD22	2.54	0.43
1:B:147:KCX:OQ1	1:B:183:HIS:HB2	2.19	0.43
1:B:313:HIS:CD2	1:B:338:LEU:HD22	2.53	0.43
1:C:147:KCX:OQ1	1:C:183:HIS:HB2	2.19	0.43
1:D:275:ALA:HA	1:D:282:MET:CE	2.47	0.43
1:B:434:ALA:HA	1:B:438:GLU:O	2.17	0.43
1:C:275:ALA:HA	1:C:282:MET:CE	2.47	0.43
1:D:55:GLY:HA3	1:D:88:THR:OG1	2.19	0.43
1:D:147:KCX:OQ1	1:D:183:HIS:HB2	2.19	0.43
1:B:55:GLY:HA3	1:B:88:THR:OG1	2.19	0.43
1:B:396:ILE:CG2	1:B:397:ASP:N	2.81	0.43
1:A:147:KCX:OQ1	1:A:183:HIS:HB2	2.19	0.42
1:A:389:LEU:HD22	1:A:427:MET:HG2	2.01	0.42
1:B:222:GLN:HE21	1:B:222:GLN:HB2	1.50	0.42
1:D:129:PRO:HB3	1:D:165:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLU:CD	1:B:76:GLU:H	2.27	0.42
1:D:243:PRO:HD3	1:D:293:MET:HB3	2.00	0.42
1:D:285:ALA:HA	1:D:286:PRO:C	2.42	0.42
1:A:76:GLU:CD	1:A:76:GLU:H	2.27	0.42
1:A:278:ILE:HB	1:A:282:MET:HE2	2.00	0.42
1:C:322:GLU:OE1	1:C:322:GLU:HA	2.20	0.42
1:D:228:GLN:NE2	1:D:233:CYS:O	2.53	0.42
1:A:215:PHE:CD1	1:A:215:PHE:C	2.98	0.42
1:B:215:PHE:CD1	1:B:215:PHE:C	2.98	0.42
1:B:275:ALA:HA	1:B:282:MET:CE	2.47	0.42
1:C:76:GLU:CD	1:C:76:GLU:H	2.27	0.42
1:C:89:THR:CG2	3:C:2022:HOH:O	2.68	0.42
1:C:129:PRO:HB3	1:C:165:GLU:OE1	2.19	0.42
1:D:89:THR:CG2	3:D:2021:HOH:O	2.68	0.42
1:B:243:PRO:HD3	1:B:293:MET:HB3	2.00	0.42
1:C:389:LEU:HD22	1:C:427:MET:HG2	2.00	0.42
1:C:398:THR:HG23	1:C:419:VAL:HB	2.01	0.42
1:D:63:ILE:N	1:D:92:GLU:OE2	2.34	0.42
1:A:6:VAL:HG21	1:A:389:LEU:HD21	2.02	0.42
1:B:129:PRO:HB3	1:B:165:GLU:OE1	2.19	0.42
1:B:274:ASP:O	1:B:282:MET:HE1	2.20	0.42
1:B:398:THR:HG23	1:B:419:VAL:HB	2.01	0.42
1:C:102:THR:HG22	1:C:103:LEU:N	2.35	0.42
1:D:76:GLU:CD	1:D:76:GLU:H	2.27	0.42
1:A:89:THR:HG21	1:A:378:LYS:CD	2.50	0.42
1:A:307:ASP:O	1:A:367:LYS:HD3	2.20	0.42
1:B:375:TYR:CB	1:B:376:PRO:CD	2.98	0.42
1:B:389:LEU:HD22	1:B:427:MET:HG2	2.01	0.42
1:D:398:THR:HG23	1:D:419:VAL:HB	2.01	0.42
1:A:33:SER:HB2	1:B:31:ALA:CB	2.46	0.42
1:A:274:ASP:O	1:A:282:MET:HE1	2.20	0.42
1:A:228:GLN:NE2	1:A:233:CYS:O	2.53	0.41
1:A:375:TYR:CB	1:A:376:PRO:CD	2.98	0.41
1:B:98:PRO:HA	1:B:99:PRO:HD3	1.92	0.41
1:C:412:SER:HA	1:C:413:PRO:HD3	1.93	0.41
1:B:234:ARG:HG3	1:B:234:ARG:NH1	2.36	0.41
1:D:89:THR:HG21	1:D:378:LYS:CD	2.50	0.41
1:A:234:ARG:HG3	1:A:234:ARG:NH1	2.36	0.41
1:B:6:VAL:HG21	1:B:389:LEU:HD21	2.02	0.41
1:B:412:SER:HA	1:B:413:PRO:HD3	1.93	0.41
1:C:149:MET:HE2	1:C:158:PHE:HD2	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ASP:O	1:C:282:MET:HE1	2.20	0.41
1:A:275:ALA:HA	1:A:282:MET:CE	2.47	0.41
1:D:102:THR:HG22	1:D:103:LEU:N	2.35	0.41
1:D:322:GLU:HA	1:D:322:GLU:OE1	2.19	0.41
1:A:149:MET:HE2	1:A:158:PHE:HD2	1.82	0.41
1:A:360:LEU:HD23	1:A:360:LEU:C	2.46	0.41
1:B:89:THR:CG2	3:B:2021:HOH:O	2.68	0.41
1:B:360:LEU:C	1:B:360:LEU:HD23	2.46	0.41
1:C:6:VAL:HG21	1:C:389:LEU:HD21	2.02	0.41
1:C:89:THR:HG21	1:C:378:LYS:CD	2.50	0.41
1:C:215:PHE:CD1	1:C:215:PHE:C	2.98	0.41
1:D:6:VAL:HG21	1:D:389:LEU:HD21	2.02	0.41
1:D:307:ASP:O	1:D:367:LYS:HD3	2.20	0.41
1:A:102:THR:HG22	1:A:103:LEU:N	2.35	0.41
1:A:322:GLU:OE1	1:A:322:GLU:HA	2.20	0.41
1:B:271:THR:CG2	1:B:273:ASP:H	2.18	0.41
1:D:215:PHE:CD1	1:D:215:PHE:C	2.98	0.41
1:D:274:ASP:O	1:D:282:MET:HE1	2.20	0.41
1:A:89:THR:CG2	3:A:2017:HOH:O	2.68	0.41
1:B:102:THR:HG22	1:B:103:LEU:N	2.35	0.41
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.83	0.41
1:C:360:LEU:HD23	1:C:360:LEU:C	2.46	0.41
1:D:389:LEU:HD22	1:D:427:MET:HG2	2.01	0.41
1:A:317:PRO:HA	1:A:409:HIS:CE1	2.56	0.41
1:B:243:PRO:HB2	1:B:296:ARG:NH2	2.36	0.41
1:B:307:ASP:O	1:B:367:LYS:HD3	2.20	0.41
1:C:307:ASP:O	1:C:367:LYS:HD3	2.20	0.41
1:C:317:PRO:HA	1:C:409:HIS:CE1	2.56	0.41
1:D:238:LEU:O	1:D:239:HIS:C	2.64	0.41
1:D:279:GLY:HA3	1:D:280:PRO:HD2	1.91	0.41
1:D:389:LEU:N	1:D:389:LEU:HD13	2.36	0.41
1:B:228:GLN:NE2	1:B:233:CYS:O	2.53	0.41
1:B:322:GLU:HA	1:B:322:GLU:OE1	2.20	0.41
1:C:228:GLN:NE2	1:C:233:CYS:O	2.53	0.41
1:C:275:ALA:CA	1:C:282:MET:HE1	2.50	0.41
1:C:279:GLY:HA3	1:C:280:PRO:HD2	1.92	0.41
1:C:375:TYR:CB	1:C:376:PRO:CD	2.98	0.41
1:D:360:LEU:HD23	1:D:360:LEU:C	2.46	0.41
1:A:238:LEU:O	1:A:239:HIS:C	2.64	0.41
1:B:389:LEU:HD13	1:B:389:LEU:N	2.36	0.40
1:C:338:LEU:HD12	1:C:338:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:THR:HG21	1:B:378:LYS:CD	2.50	0.40
1:B:238:LEU:O	1:B:239:HIS:C	2.64	0.40
1:C:234:ARG:HG3	1:C:234:ARG:NH1	2.36	0.40
1:C:450:THR:OG1	1:C:451:ARG:N	2.52	0.40
1:D:275:ALA:CA	1:D:282:MET:HE1	2.50	0.40
1:D:451:ARG:NH1	1:D:451:ARG:CG	2.84	0.40
1:C:278:ILE:HB	1:C:282:MET:HE2	2.00	0.40
1:D:412:SER:HA	1:D:413:PRO:HD3	1.93	0.40
1:A:389:LEU:HD13	1:A:389:LEU:N	2.36	0.40
1:C:367:LYS:O	1:C:368:PRO:C	2.64	0.40
1:D:234:ARG:HG3	1:D:234:ARG:NH1	2.36	0.40
1:A:324:GLY:HA3	1:A:331:ALA:HB2	2.04	0.40
1:B:228:GLN:HG3	1:B:229:LYS:N	2.37	0.40
1:B:324:GLY:HA3	1:B:331:ALA:HB2	2.04	0.40
1:D:317:PRO:HA	1:D:409:HIS:CE1	2.56	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:GLU:OE2	1:D:71:ARG:NH2[2_645]	1.40	0.80
1:A:319:GLU:OE2	1:C:71:ARG:NH2[2_554]	1.48	0.72
1:B:159:ASP:OD2	1:D:326:LYS:NZ[2_645]	1.50	0.70
1:A:159:ASP:OD2	1:C:326:LYS:NZ[2_554]	1.92	0.28
3:B:2014:HOH:O	3:D:2114:HOH:O[2_645]	1.93	0.27
1:B:319:GLU:CD	1:D:71:ARG:NH2[2_645]	1.99	0.21
1:B:71:ARG:CD	1:D:319:GLU:OE2[2_645]	2.17	0.03
1:B:319:GLU:CG	1:D:71:ARG:NH2[2_645]	2.18	0.02

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	448/458 (98%)	418 (93%)	26 (6%)	4 (1%)	14	30
1	B	448/458 (98%)	418 (93%)	26 (6%)	4 (1%)	14	30
1	C	448/458 (98%)	418 (93%)	26 (6%)	4 (1%)	14	30
1	D	448/458 (98%)	418 (93%)	26 (6%)	4 (1%)	14	30
All	All	1792/1832 (98%)	1672 (93%)	104 (6%)	16 (1%)	14	30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	TYR
1	B	375	TYR
1	C	375	TYR
1	D	375	TYR
1	A	239	HIS
1	B	239	HIS
1	C	239	HIS
1	D	239	HIS
1	A	337	GLY
1	B	337	GLY
1	C	337	GLY
1	D	337	GLY
1	A	376	PRO
1	B	376	PRO
1	C	376	PRO
1	D	376	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	367/373 (98%)	325 (89%)	42 (11%)	5	11
1	B	367/373 (98%)	325 (89%)	42 (11%)	5	11
1	C	367/373 (98%)	325 (89%)	42 (11%)	5	11
1	D	367/373 (98%)	325 (89%)	42 (11%)	5	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1468/1492 (98%)	1300 (89%)	168 (11%)	5 11

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	23	LEU
1	A	24	VAL
1	A	28	LYS
1	A	33	SER
1	A	44	THR
1	A	76	GLU
1	A	89	THR
1	A	93	MET
1	A	107	LEU
1	A	188	THR
1	A	222	GLN
1	A	225	LEU
1	A	228	GLN
1	A	247	GLU
1	A	248	LEU
1	A	266	GLN
1	A	271	THR
1	A	273	ASP
1	A	289	ARG
1	A	297	LEU
1	A	301	LEU
1	A	309	LEU
1	A	316	HIS
1	A	322	GLU
1	A	338	LEU
1	A	342	LEU
1	A	344	MET
1	A	346	LEU
1	A	354	ARG
1	A	381	LEU
1	A	389	LEU
1	A	394	LEU
1	A	400	VAL
1	A	425	LEU
1	A	426	THR
1	A	428	VAL

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Mol	Chain	Res	Type
1	A	431	THR
1	A	441	VAL
1	A	442	GLU
1	A	449	VAL
1	A	451	ARG
1	B	12	VAL
1	B	23	LEU
1	B	24	VAL
1	B	28	LYS
1	B	33	SER
1	B	44	THR
1	B	76	GLU
1	B	89	THR
1	B	93	MET
1	B	107	LEU
1	B	188	THR
1	B	222	GLN
1	B	225	LEU
1	B	228	GLN
1	B	247	GLU
1	B	248	LEU
1	B	266	GLN
1	B	271	THR
1	B	273	ASP
1	B	289	ARG
1	B	297	LEU
1	B	301	LEU
1	B	309	LEU
1	B	316	HIS
1	B	322	GLU
1	B	338	LEU
1	B	342	LEU
1	B	344	MET
1	B	346	LEU
1	B	354	ARG
1	B	381	LEU
1	B	389	LEU
1	B	394	LEU
1	B	400	VAL
1	B	425	LEU
1	B	426	THR
1	B	428	VAL

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Mol	Chain	Res	Type
1	B	431	THR
1	B	441	VAL
1	B	442	GLU
1	B	449	VAL
1	B	451	ARG
1	C	12	VAL
1	C	23	LEU
1	C	24	VAL
1	C	28	LYS
1	C	33	SER
1	C	44	THR
1	C	76	GLU
1	C	89	THR
1	C	93	MET
1	C	107	LEU
1	C	188	THR
1	C	222	GLN
1	C	225	LEU
1	C	228	GLN
1	C	247	GLU
1	C	248	LEU
1	C	266	GLN
1	C	271	THR
1	C	273	ASP
1	C	289	ARG
1	C	297	LEU
1	C	301	LEU
1	C	309	LEU
1	C	316	HIS
1	C	322	GLU
1	C	338	LEU
1	C	342	LEU
1	C	344	MET
1	C	346	LEU
1	C	354	ARG
1	C	381	LEU
1	C	389	LEU
1	C	394	LEU
1	C	400	VAL
1	C	425	LEU
1	C	426	THR
1	C	428	VAL

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Mol	Chain	Res	Type
1	C	431	THR
1	C	441	VAL
1	C	442	GLU
1	C	449	VAL
1	C	451	ARG
1	D	12	VAL
1	D	23	LEU
1	D	24	VAL
1	D	28	LYS
1	D	33	SER
1	D	44	THR
1	D	76	GLU
1	D	89	THR
1	D	93	MET
1	D	107	LEU
1	D	188	THR
1	D	222	GLN
1	D	225	LEU
1	D	228	GLN
1	D	247	GLU
1	D	248	LEU
1	D	266	GLN
1	D	271	THR
1	D	273	ASP
1	D	289	ARG
1	D	297	LEU
1	D	301	LEU
1	D	309	LEU
1	D	316	HIS
1	D	322	GLU
1	D	338	LEU
1	D	342	LEU
1	D	344	MET
1	D	346	LEU
1	D	354	ARG
1	D	381	LEU
1	D	389	LEU
1	D	394	LEU
1	D	400	VAL
1	D	425	LEU
1	D	426	THR
1	D	428	VAL

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Mol	Chain	Res	Type
1	D	431	THR
1	D	441	VAL
1	D	442	GLU
1	D	449	VAL
1	D	451	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	171	GLN
1	A	191	GLN
1	A	194	GLN
1	A	196	GLN
1	A	212	GLN
1	A	218	ASN
1	A	228	GLN
1	A	253	GLN
1	A	257	GLN
1	A	266	GLN
1	A	316	HIS
1	A	382	GLN
1	A	447	GLN
1	B	115	GLN
1	B	171	GLN
1	B	191	GLN
1	B	194	GLN
1	B	212	GLN
1	B	218	ASN
1	B	228	GLN
1	B	253	GLN
1	B	257	GLN
1	B	266	GLN
1	B	316	HIS
1	B	382	GLN
1	B	447	GLN
1	C	115	GLN
1	C	171	GLN
1	C	191	GLN
1	C	194	GLN
1	C	196	GLN
1	C	212	GLN

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Mol	Chain	Res	Type
1	C	218	ASN
1	C	222	GLN
1	C	228	GLN
1	C	251	GLN
1	C	253	GLN
1	C	257	GLN
1	C	266	GLN
1	C	316	HIS
1	C	382	GLN
1	C	447	GLN
1	D	115	GLN
1	D	191	GLN
1	D	194	GLN
1	D	196	GLN
1	D	212	GLN
1	D	218	ASN
1	D	222	GLN
1	D	228	GLN
1	D	251	GLN
1	D	253	GLN
1	D	257	GLN
1	D	266	GLN
1	D	316	HIS
1	D	382	GLN
1	D	447	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	KCX	C	147	1,2	10,11,12	1.06	0	6,12,14	2.11	1 (16%)
1	KCX	D	147	1,2	10,11,12	1.06	0	6,12,14	2.13	1 (16%)
1	KCX	B	147	1,2	10,11,12	1.05	0	6,12,14	2.12	1 (16%)
1	KCX	A	147	1,2	10,11,12	1.06	1 (10%)	6,12,14	2.12	1 (16%)

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
1	KCX	C	147	1,2	-	3/9/10/12	-
1	KCX	D	147	1,2	-	3/9/10/12	-
1	KCX	B	147	1,2	-	3/9/10/12	-
1	KCX	A	147	1,2	-	3/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	KCX	OQ1-CX	2.02	1.25	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	KCX	OQ1-CX-NZ	-4.88	117.50	124.92
1	A	147	KCX	OQ1-CX-NZ	-4.87	117.52	124.92
1	B	147	KCX	OQ1-CX-NZ	-4.86	117.54	124.92
1	C	147	KCX	OQ1-CX-NZ	-4.86	117.55	124.92

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	147	KCX	O-C-CA-CB
1	B	147	KCX	O-C-CA-CB
1	C	147	KCX	O-C-CA-CB
1	D	147	KCX	O-C-CA-CB
1	A	147	KCX	CE-CD-CG-CB
1	C	147	KCX	CE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
1	D	147	KCX	CE-CD-CG-CB
1	B	147	KCX	CE-CD-CG-CB
1	A	147	KCX	CG-CD-CE-NZ
1	B	147	KCX	CG-CD-CE-NZ
1	C	147	KCX	CG-CD-CE-NZ
1	D	147	KCX	CG-CD-CE-NZ

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	147	KCX	3	0
1	D	147	KCX	3	0
1	B	147	KCX	3	0
1	A	147	KCX	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	450/458 (98%)	0.42	31 (6%)	23	18	5, 20, 44, 76	0
1	B	450/458 (98%)	0.38	31 (6%)	23	18	5, 20, 44, 76	0
1	C	450/458 (98%)	0.32	32 (7%)	22	17	5, 20, 44, 76	0
1	D	450/458 (98%)	0.25	16 (3%)	46	40	5, 20, 44, 76	0
All	All	1800/1832 (98%)	0.34	110 (6%)	27	22	5, 20, 45, 76	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	155	PRO	6.3
1	C	315	GLY	6.3
1	C	68	LEU	5.9
1	A	318	VAL	5.7
1	A	156	GLY	5.6
1	C	71	ARG	5.6
1	C	153	SER	5.3
1	B	71	ARG	5.2
1	C	156	GLY	5.0
1	A	71	ARG	4.6
1	A	154	VAL	4.6
1	C	154	VAL	4.5
1	C	157	MET	4.3
1	B	38	ASP	4.2
1	A	320	ASP	4.1
1	B	153	SER	4.1
1	A	38	ASP	4.1
1	A	319	GLU	4.0
1	D	156	GLY	4.0
1	D	71	ARG	4.0
1	D	153	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	319	GLU	3.8
1	A	1	MET	3.8
1	A	70	ASN	3.7
1	A	157	MET	3.6
1	A	155	PRO	3.6
1	B	1	MET	3.5
1	D	157	MET	3.5
1	B	320	ASP	3.5
1	C	442	GLU	3.5
1	D	155	PRO	3.3
1	C	324	GLY	3.3
1	B	154	VAL	3.2
1	C	319	GLU	3.2
1	C	375	TYR	3.2
1	C	318	VAL	3.1
1	D	317	PRO	3.1
1	C	316	HIS	3.1
1	C	72	TYR	3.0
1	B	152	ALA	3.0
1	B	442	GLU	3.0
1	B	37	SER	3.0
1	D	154	VAL	2.9
1	A	376	PRO	2.9
1	A	332	GLY	2.9
1	B	330	LYS	2.8
1	D	152	ALA	2.8
1	C	152	ALA	2.8
1	B	332	GLY	2.7
1	B	375	TYR	2.7
1	C	70	ASN	2.7
1	B	157	MET	2.6
1	B	40	GLU	2.6
1	B	155	PRO	2.6
1	A	37	SER	2.5
1	B	204	ASP	2.5
1	C	314	GLY	2.5
1	D	1	MET	2.5
1	C	273	ASP	2.5
1	B	318	VAL	2.5
1	D	319	GLU	2.5
1	A	152	ALA	2.5
1	C	331	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	74	ARG	2.4
1	C	204	ASP	2.4
1	A	292	GLU	2.4
1	C	332	GLY	2.4
1	D	318	VAL	2.4
1	D	38	ASP	2.4
1	A	39	VAL	2.4
1	A	74	ARG	2.4
1	B	36	THR	2.4
1	A	316	HIS	2.4
1	C	326	LYS	2.4
1	A	375	TYR	2.3
1	C	317	PRO	2.3
1	D	315	GLY	2.3
1	B	68	LEU	2.3
1	B	254	SER	2.3
1	B	156	GLY	2.3
1	B	222	GLN	2.3
1	B	7	LYS	2.3
1	A	317	PRO	2.3
1	B	39	VAL	2.3
1	A	202	GLY	2.2
1	C	37	SER	2.2
1	C	320	ASP	2.2
1	C	1	MET	2.2
1	C	36	THR	2.2
1	A	442	GLU	2.1
1	A	326	LYS	2.1
1	B	72	TYR	2.1
1	A	199	ALA	2.1
1	B	276	GLU	2.1
1	B	322	GLU	2.1
1	A	153	SER	2.1
1	B	43	ARG	2.1
1	B	329	TRP	2.1
1	C	136	ARG	2.1
1	A	195	LYS	2.1
1	A	315	GLY	2.1
1	C	328	VAL	2.1
1	A	273	ASP	2.1
1	B	273	ASP	2.1
1	C	406	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	376	PRO	2.1
1	D	275	ALA	2.0
1	D	437	GLY	2.0
1	A	104	ASP	2.0
1	A	68	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	D	147	12/13	0.90	0.11	5,9,12,15	0
1	KCX	B	147	12/13	0.92	0.11	5,9,12,15	0
1	KCX	A	147	12/13	0.92	0.11	5,9,12,15	0
1	KCX	C	147	12/13	0.93	0.09	5,9,12,15	0

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	ZN	C	1452	1/1	0.94	0.05	19,19,19,19	0
2	ZN	B	1453	1/1	0.96	0.06	17,17,17,17	0
2	ZN	D	1452	1/1	0.96	0.04	19,19,19,19	0
2	ZN	B	1452	1/1	0.97	0.06	19,19,19,19	0
2	ZN	C	1453	1/1	0.98	0.05	17,17,17,17	0
2	ZN	A	1452	1/1	0.98	0.07	19,19,19,19	0
2	ZN	A	1453	1/1	0.99	0.07	17,17,17,17	0
2	ZN	D	1453	1/1	0.99	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.