



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:26 PM UTC

PDB ID : 5IMH / pdb_00005imh
Title : D31P mutant of C69-family cysteine dipeptidase from *Lactobacillus farciminis*
Authors : Kono, R.; Watanabe, K.
Deposited on : 2016-03-06
Resolution : 2.47 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

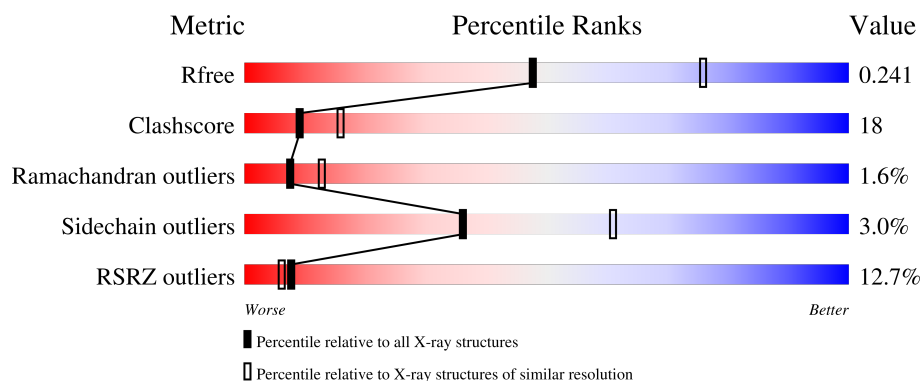
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	469	12% 72% 22% 5%
1	B	469	13% 72% 21% 5%
1	C	469	13% 71% 21% 5%
1	D	469	13% 74% 21% 5%
1	E	469	13% 71% 20% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19121 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 Dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3706	2323	631	740	12			
1	B	467	Total	C	N	O	S	0	0	0
			3706	2323	631	740	12			
1	C	467	Total	C	N	O	S	0	0	0
			3706	2323	631	740	12			
1	D	467	Total	C	N	O	S	0	0	0
			3706	2323	631	740	12			
1	E	467	Total	C	N	O	S	0	0	0
			3706	2323	631	740	12			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	PRO	ASP	engineered mutation	UNP A0A0R1IQH8
B	31	PRO	ASP	engineered mutation	UNP A0A0R1IQH8
C	31	PRO	ASP	engineered mutation	UNP A0A0R1IQH8
D	31	PRO	ASP	engineered mutation	UNP A0A0R1IQH8
E	31	PRO	ASP	engineered mutation	UNP A0A0R1IQH8

- Molecule 2 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Co	0	0
			2	2		
2	B	1	Total	Co	0	0
			1	1		
2	C	2	Total	Co	0	0
			2	2		
2	D	1	Total	Co	0	0
			1	1		
2	E	1	Total	Co	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

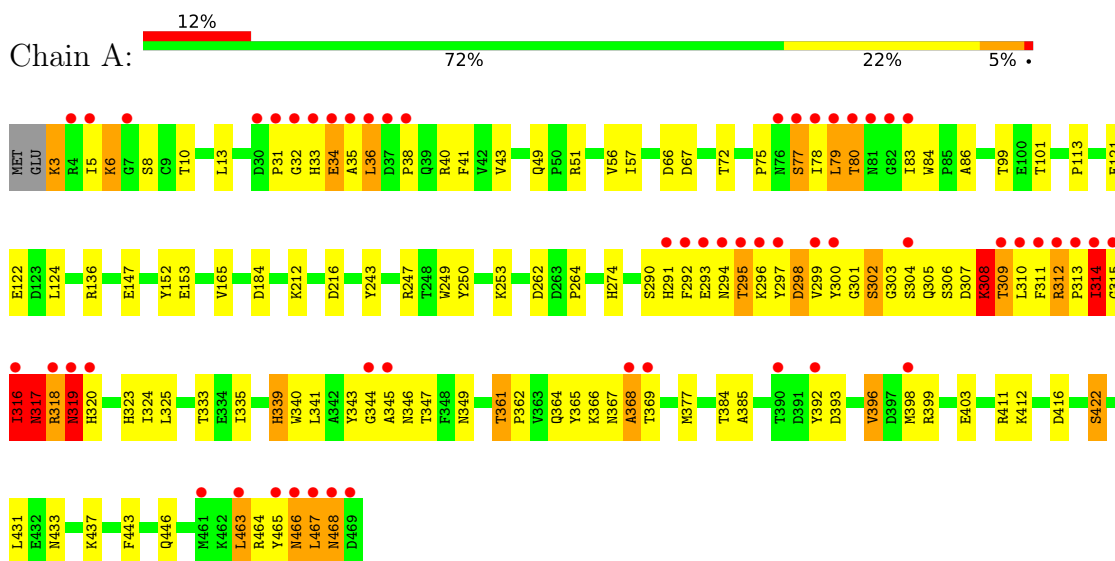
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	159	Total	O	0	0
			159	159		
5	B	114	Total	O	0	0
			114	114		
5	C	107	Total	O	0	0
			107	107		
5	D	97	Total	O	0	0
			97	97		
5	E	83	Total	O	0	0
			83	83		

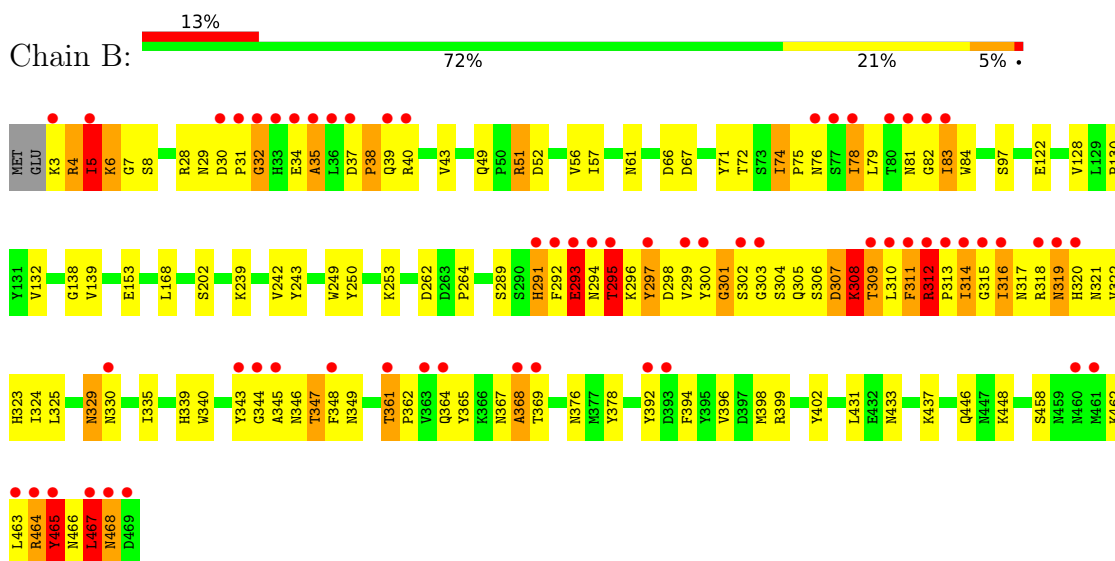
3 Residue-property plots

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.

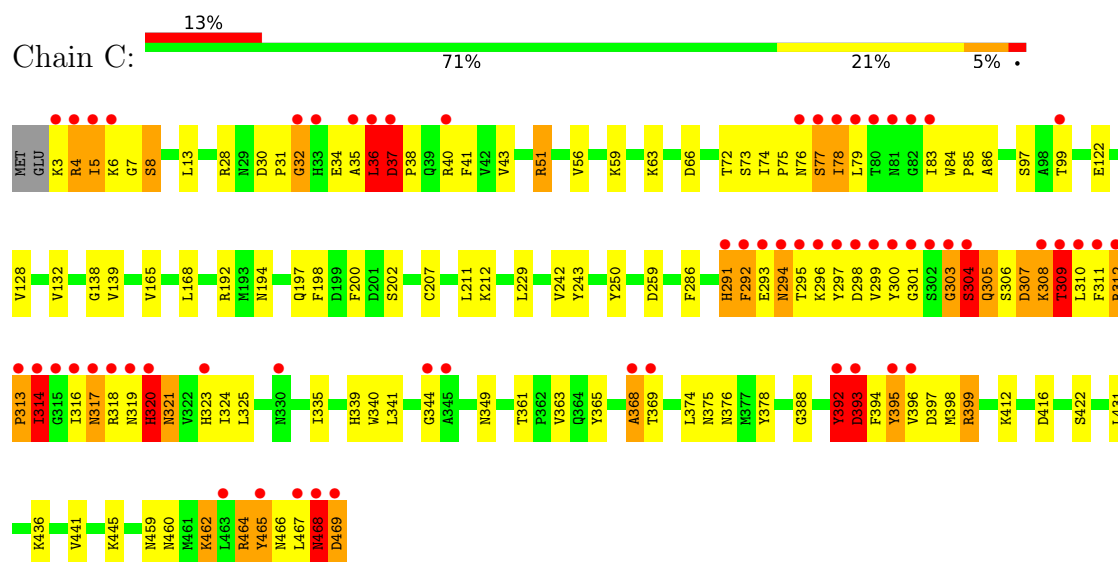
• Molecule 1: Dipeptidase



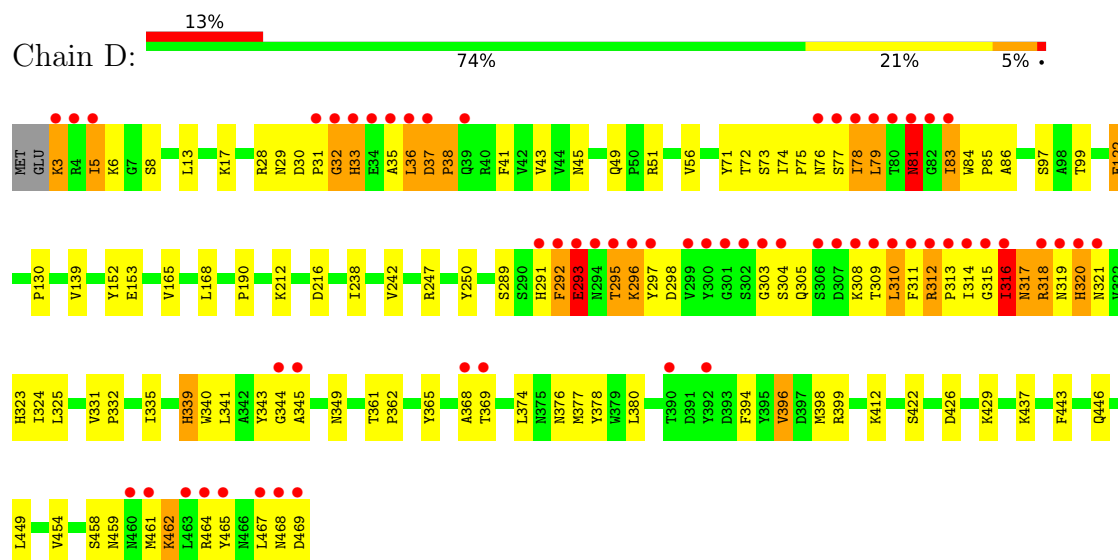
• Molecule 1: Dipeptidase



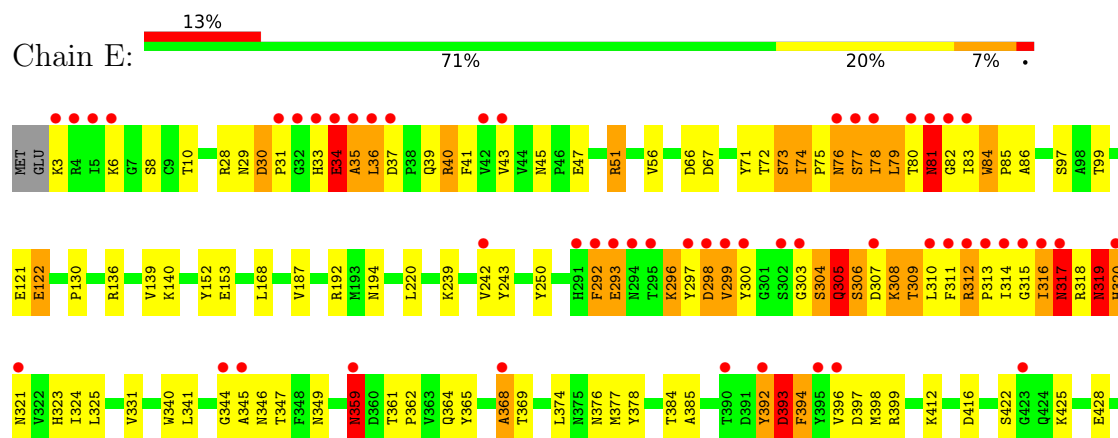
• Molecule 1: Dipeptidase

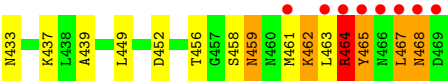


• Molecule 1: Dipeptidase



• Molecule 1: Dipeptidase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	192.34Å 137.09Å 101.30Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	47.24 – 2.47 47.24 – 2.47	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.24-2.47) 99.4 (47.24-2.47)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.96 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.188 , 0.240 0.193 , 0.241	Depositor DCC
R_{free} test set	4624 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19121	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: EDO, CO, ACT

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	0.69	0/3789	1.15	20/5157 (0.4%)
1	B	0.71	1/3789 (0.0%)	1.24	40/5157 (0.8%)
1	C	0.70	2/3789 (0.1%)	1.18	41/5157 (0.8%)
1	D	0.64	0/3789	1.12	29/5157 (0.6%)
1	E	0.69	2/3789 (0.1%)	1.24	48/5157 (0.9%)
All	All	0.68	5/18945 (0.0%)	1.19	178/25785 (0.7%)

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	3
1	B	0	3
1	C	0	7
1	D	0	3
1	E	0	12
All	All	0	28

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	ILE	CA-CB	6.18	1.62	1.54
1	C	314	ILE	CA-CB	6.17	1.62	1.54
1	E	462	LYS	CD-CE	-5.91	1.34	1.52
1	C	309	THR	CA-CB	5.78	1.63	1.53
1	E	462	LYS	CA-CB	-5.70	1.43	1.53

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	312	ARG	CA-C-N	15.45	139.16	119.84
1	B	312	ARG	C-N-CA	15.45	139.16	119.84
1	B	302	SER	N-CA-C	14.15	126.70	111.28
1	A	308	LYS	N-CA-C	13.28	129.25	109.07
1	C	312	ARG	CA-C-N	11.79	134.58	119.84
1	C	312	ARG	C-N-CA	11.79	134.58	119.84
1	A	312	ARG	CA-C-N	11.16	131.87	119.93
1	A	312	ARG	C-N-CA	11.16	131.87	119.93
1	B	307	ASP	N-CA-C	-10.54	101.13	112.93
1	C	393	ASP	N-CA-C	10.22	124.58	107.20
1	E	308	LYS	CA-CB-CG	-10.21	93.68	114.10
1	D	317	ASN	CA-C-N	9.85	139.42	121.70
1	D	317	ASN	C-N-CA	9.85	139.42	121.70
1	E	74	ILE	CA-C-N	9.74	132.02	119.84
1	E	74	ILE	C-N-CA	9.74	132.02	119.84
1	E	36	LEU	CA-CB-CG	9.63	150.02	116.30
1	A	302	SER	N-CA-C	9.37	124.27	113.02
1	B	74	ILE	CA-C-N	9.31	131.48	119.84
1	B	74	ILE	C-N-CA	9.31	131.48	119.84
1	A	294	ASN	N-CA-C	-9.04	96.53	108.19
1	C	468	ASN	N-CA-C	8.86	129.68	110.80
1	A	464	ARG	N-CA-C	-8.76	102.60	113.28
1	A	317	ASN	N-CA-C	8.68	124.51	114.62
1	E	30	ASP	CA-C-N	-8.59	109.11	119.84
1	E	30	ASP	C-N-CA	-8.59	109.11	119.84
1	D	310	LEU	N-CA-C	8.51	123.21	111.55
1	E	80	THR	N-CA-C	-8.47	103.08	113.41
1	B	464	ARG	N-CA-C	-8.45	102.97	113.20
1	D	317	ASN	N-CA-CB	-8.44	97.22	111.31
1	C	395	TYR	N-CA-C	8.39	124.54	113.30
1	B	293	GLU	N-CA-C	8.35	122.62	108.02
1	B	329	ASN	N-CA-C	-8.30	93.13	110.80
1	D	394	PHE	N-CA-C	-8.29	103.35	113.97
1	A	468	ASN	N-CA-C	8.21	128.28	110.80
1	E	394	PHE	N-CA-C	-8.14	103.14	113.72
1	D	38	PRO	CA-C-N	-8.01	111.95	123.00
1	D	38	PRO	C-N-CA	-8.01	111.95	123.00
1	D	293	GLU	N-CA-C	8.00	123.38	107.62
1	D	317	ASN	CA-C-O	-7.91	112.62	121.40
1	C	78	ILE	N-CA-C	7.89	121.59	109.12
1	C	467	LEU	N-CA-C	7.85	123.15	109.80
1	C	306	SER	N-CA-C	-7.55	103.87	113.23
1	B	368	ALA	CA-C-N	7.45	135.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	ALA	C-N-CA	7.45	135.10	121.70
1	C	294	ASN	N-CA-CB	7.43	117.09	109.51
1	A	306	SER	N-CA-C	-7.42	103.63	114.39
1	E	36	LEU	CB-CG-CD2	7.41	132.94	110.70
1	B	467	LEU	N-CA-C	7.37	126.49	110.80
1	E	462	LYS	CD-CE-NZ	-7.32	88.47	111.90
1	E	81	ASN	N-CA-C	7.32	126.39	110.80
1	E	468	ASN	N-CA-C	7.30	120.51	109.41
1	E	308	LYS	CB-CG-CD	7.30	128.09	111.30
1	E	37	ASP	CA-C-N	-7.23	111.59	119.98
1	E	37	ASP	C-N-CA	-7.23	111.59	119.98
1	A	34	GLU	N-CA-C	-7.21	95.44	110.80
1	E	307	ASP	N-CA-C	-7.19	104.66	113.50
1	C	7	GLY	N-CA-C	7.17	130.16	113.18
1	C	5	ILE	N-CA-C	7.14	119.41	109.55
1	C	8	SER	N-CA-C	7.05	120.17	108.96
1	C	393	ASP	CA-C-O	7.05	127.21	120.09
1	B	301	GLY	N-CA-C	7.03	129.85	113.18
1	C	307	ASP	N-CA-C	6.99	120.69	112.72
1	E	303	GLY	N-CA-C	6.81	126.30	111.04
1	E	76	ASN	N-CA-C	6.78	125.24	110.80
1	E	293	GLU	N-CA-C	6.77	120.96	107.62
1	E	462	LYS	CB-CG-CD	-6.75	95.77	111.30
1	A	310	LEU	N-CA-C	6.71	120.37	112.72
1	B	394	PHE	N-CA-C	-6.69	105.41	113.97
1	E	79	LEU	N-CA-C	6.65	116.64	107.73
1	A	466	ASN	N-CA-C	6.64	119.11	108.41
1	D	305	GLN	N-CA-C	-6.63	103.34	112.03
1	D	296	LYS	N-CA-C	6.63	123.42	110.56
1	B	347	THR	N-CA-C	-6.60	105.11	113.02
1	D	461	MET	N-CA-C	-6.58	104.14	111.71
1	E	35	ALA	N-CA-C	6.43	124.50	110.80
1	E	368	ALA	CA-C-N	6.41	133.25	121.70
1	E	368	ALA	C-N-CA	6.41	133.25	121.70
1	B	38	PRO	CA-C-N	-6.41	114.16	123.00
1	B	38	PRO	C-N-CA	-6.41	114.16	123.00
1	B	128	VAL	CB-CA-C	-6.36	106.31	111.71
1	B	5	ILE	N-CA-C	6.27	122.39	109.34
1	D	78	ILE	N-CA-C	6.27	118.39	108.87
1	E	298	ASP	N-CA-C	6.26	118.97	109.95
1	E	36	LEU	N-CA-C	6.23	119.69	110.48
1	E	77	SER	N-CA-C	6.18	123.97	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	LYS	CD-CE-NZ	-6.16	92.19	111.90
1	B	311	PHE	N-CA-C	-6.14	99.19	109.07
1	C	397	ASP	N-CA-C	-6.13	104.50	112.23
1	E	392	TYR	N-CA-C	6.13	118.76	111.71
1	B	37	ASP	CA-C-N	-6.03	111.59	120.46
1	B	37	ASP	C-N-CA	-6.03	111.59	120.46
1	C	459	ASN	N-CA-C	-6.03	105.97	113.38
1	E	312	ARG	CA-C-N	6.02	126.37	119.93
1	E	312	ARG	C-N-CA	6.02	126.37	119.93
1	D	37	ASP	N-CA-C	5.95	122.96	109.81
1	E	36	LEU	CB-CG-CD1	-5.93	92.92	110.70
1	A	368	ALA	CA-C-N	5.92	132.35	121.70
1	A	368	ALA	C-N-CA	5.92	132.35	121.70
1	C	32	GLY	N-CA-C	-5.92	101.10	111.46
1	C	392	TYR	CA-C-N	-5.89	113.09	121.33
1	C	392	TYR	C-N-CA	-5.89	113.09	121.33
1	D	317	ASN	CB-CA-C	5.88	125.77	111.65
1	D	292	PHE	CA-C-N	-5.88	114.44	123.14
1	D	292	PHE	C-N-CA	-5.88	114.44	123.14
1	B	78	ILE	N-CA-C	5.83	117.14	109.21
1	C	308	LYS	CA-C-N	5.82	132.66	121.54
1	C	308	LYS	C-N-CA	5.82	132.66	121.54
1	D	320	HIS	N-CA-C	5.80	119.04	107.62
1	C	321	ASN	N-CA-C	-5.79	98.30	108.20
1	C	467	LEU	CA-C-N	5.76	132.54	121.54
1	C	467	LEU	C-N-CA	5.76	132.54	121.54
1	B	301	GLY	CA-C-N	5.75	127.98	120.28
1	B	301	GLY	C-N-CA	5.75	127.98	120.28
1	D	298	ASP	N-CA-C	5.74	118.60	109.81
1	A	319	ASN	N-CA-C	-5.73	100.44	109.50
1	E	331	VAL	N-CA-C	-5.73	102.53	109.01
1	B	295	THR	N-CA-C	5.72	122.98	110.80
1	A	307	ASP	N-CA-C	-5.69	105.92	112.92
1	D	462	LYS	N-CA-C	-5.65	105.03	111.14
1	C	304	SER	N-CA-C	5.65	126.81	111.00
1	D	81	ASN	N-CA-C	5.63	122.80	110.80
1	E	422	SER	N-CA-C	5.60	117.39	111.28
1	B	309	THR	N-CA-C	5.59	122.71	110.80
1	D	312	ARG	CA-C-N	5.59	125.87	119.83
1	D	312	ARG	C-N-CA	5.59	125.87	119.83
1	C	4	ARG	N-CA-C	5.59	115.49	108.45
1	C	128	VAL	CB-CA-C	-5.58	106.97	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	84	TRP	CA-C-N	5.56	125.73	119.90
1	E	84	TRP	C-N-CA	5.56	125.73	119.90
1	A	422	SER	N-CA-C	5.53	118.06	111.71
1	E	397	ASP	N-CA-C	-5.52	105.27	112.23
1	D	422	SER	N-CA-C	5.49	117.26	111.28
1	B	51	ARG	N-CA-C	-5.48	106.76	113.50
1	A	290	SER	N-CA-C	5.42	117.36	108.52
1	B	467	LEU	CA-C-N	5.39	131.84	121.54
1	B	467	LEU	C-N-CA	5.39	131.84	121.54
1	B	32	GLY	N-CA-C	-5.38	103.19	111.64
1	B	468	ASN	N-CA-C	5.37	122.23	110.80
1	D	36	LEU	CA-CB-CG	5.35	135.01	116.30
1	C	37	ASP	CA-C-N	-5.33	114.30	119.90
1	C	37	ASP	C-N-CA	-5.33	114.30	119.90
1	C	422	SER	N-CA-C	5.33	117.09	111.28
1	C	320	HIS	CA-C-N	-5.31	115.94	122.84
1	C	320	HIS	C-N-CA	-5.31	115.94	122.84
1	E	319	ASN	N-CA-C	-5.30	100.77	109.40
1	E	359	ASN	N-CA-CB	5.29	118.60	110.61
1	B	297	TYR	CA-C-N	-5.28	112.59	122.73
1	B	297	TYR	C-N-CA	-5.28	112.59	122.73
1	B	367	ASN	N-CA-C	5.28	116.81	109.31
1	A	36	LEU	CA-CB-CG	5.27	134.75	116.30
1	C	368	ALA	CA-C-N	5.26	131.17	121.70
1	C	368	ALA	C-N-CA	5.26	131.17	121.70
1	C	303	GLY	CA-C-N	5.25	131.14	121.70
1	C	303	GLY	C-N-CA	5.25	131.14	121.70
1	E	303	GLY	CA-C-N	5.24	131.14	121.70
1	E	303	GLY	C-N-CA	5.24	131.14	121.70
1	E	317	ASN	N-CA-C	-5.24	99.63	110.80
1	E	464	ARG	N-CA-C	-5.24	104.50	112.04
1	E	45	ASN	CA-C-N	5.23	125.29	119.32
1	E	45	ASN	C-N-CA	5.23	125.29	119.32
1	C	36	LEU	N-CA-C	5.21	118.06	109.72
1	B	202	SER	N-CA-C	5.17	117.79	110.50
1	C	309	THR	N-CA-CB	5.16	119.21	110.49
1	C	303	GLY	N-CA-C	5.14	125.37	113.18
1	D	35	ALA	N-CA-C	5.12	117.98	107.69
1	A	314	ILE	N-CA-C	5.11	115.63	108.17
1	E	82	GLY	N-CA-C	-5.09	106.99	111.67
1	B	312	ARG	N-CA-C	5.07	117.51	109.40
1	D	331	VAL	N-CA-C	-5.07	103.28	109.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	SER	N-CA-C	-5.07	101.70	108.34
1	E	308	LYS	CA-C-N	5.05	131.56	122.46
1	E	308	LYS	C-N-CA	5.05	131.56	122.46
1	B	307	ASP	CB-CA-C	-5.05	102.08	110.81
1	E	465	TYR	CA-CB-CG	5.04	122.98	113.90
1	B	4	ARG	N-CA-C	5.03	115.96	108.86
1	C	51	ARG	N-CA-C	-5.03	107.32	113.50
1	D	32	GLY	N-CA-C	-5.02	103.55	112.54
1	D	36	LEU	N-CA-C	-5.01	101.52	109.59

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	298	ASP	Peptide
1	A	316	ILE	Peptide
1	A	318	ARG	Peptide
1	B	293	GLU	Peptide
1	B	308	LYS	Peptide
1	B	465	TYR	Peptide
1	C	293	GLU	Peptide
1	C	304	SER	Peptide
1	C	309	THR	Peptide
1	C	392	TYR	Peptide
1	C	393	ASP	Peptide
1	C	464	ARG	Peptide
1	C	468	ASN	Peptide
1	D	293	GLU	Peptide
1	D	316	ILE	Peptide
1	D	81	ASN	Peptide
1	E	293	GLU	Peptide
1	E	304	SER	Peptide
1	E	305	GLN	Peptide
1	E	306	SER	Peptide
1	E	309	THR	Peptide
1	E	316	ILE	Peptide
1	E	317	ASN	Peptide
1	E	34	GLU	Peptide
1	E	393	ASP	Peptide
1	E	464	ARG	Peptide
1	E	81	ASN	Peptide
1	E	83	ILE	Peptide

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	3706	0	3539	131	0
1	B	3706	0	3539	161	0
1	C	3706	0	3539	147	0
1	D	3706	0	3539	110	0
1	E	3706	0	3539	127	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	12	0	18	3	0
3	C	8	0	12	2	0
4	B	4	0	3	0	0
5	A	159	0	0	8	0
5	B	114	0	0	4	0
5	C	107	0	0	5	0
5	D	97	0	0	6	0
5	E	83	0	0	1	0
All	All	19121	0	17728	664	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 18.

All (664) 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:E:297:TYR:HB3	1:E:308:LYS:HD2	1.21	1.13
1:B:317:ASN:H	1:B:318:ARG:HA	1.19	1.02
1:C:34:GLU:HG2	1:C:35:ALA:H	1.25	1.00
1:E:317:ASN:H	1:E:318:ARG:HB2	1.27	0.95
1:C:363:VAL:H	1:C:436:LYS:HZ2	1.13	0.95
1:B:318:ARG:NH1	1:B:346:ASN:O	2.01	0.92
1:B:79:LEU:HD21	1:B:84:TRP:HD1	1.34	0.92
1:E:368:ALA:HA	1:E:369:THR:HG22	1.51	0.91
1:E:308:LYS:HZ1	1:E:311:PHE:HB2	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ARG:HD2	1:C:319:ASN:HB2	1.54	0.90
1:B:368:ALA:HA	1:B:369:THR:HG22	1.55	0.89
1:C:291:HIS:CE1	1:C:316:ILE:HB	2.10	0.87
1:E:308:LYS:NZ	1:E:311:PHE:HB2	1.88	0.87
1:D:6:LYS:NZ	1:D:153:GLU:OE2	2.09	0.86
1:C:319:ASN:OD1	1:C:320:HIS:N	2.09	0.85
1:E:318:ARG:HD2	1:E:319:ASN:H	1.41	0.85
1:E:292:PHE:HD1	1:E:296:LYS:HZ1	1.23	0.85
1:B:309:THR:OG1	1:B:311:PHE:N	2.10	0.84
1:E:30:ASP:N	1:E:318:ARG:HH12	1.77	0.82
1:E:359:ASN:N	1:E:359:ASN:HD22	1.75	0.82
1:A:317:ASN:C	1:A:317:ASN:HD22	1.88	0.82
1:D:32:GLY:N	1:D:319:ASN:OD1	2.13	0.82
1:B:317:ASN:N	1:B:318:ARG:HA	1.95	0.81
1:E:297:TYR:HB3	1:E:308:LYS:CD	2.07	0.81
1:D:396:VAL:HG22	1:D:399:ARG:NH2	1.96	0.81
1:A:317:ASN:HD22	1:A:318:ARG:N	1.78	0.81
1:A:364:GLN:HG2	1:A:377:MET:HE3	1.62	0.80
1:C:298:ASP:H	1:C:308:LYS:HE2	1.45	0.80
1:C:396:VAL:HA	1:C:399:ARG:HB3	1.63	0.80
1:D:468:ASN:OD1	1:D:469:ASP:N	2.15	0.80
1:B:30:ASP:HB3	1:B:321:ASN:HB2	1.63	0.80
1:D:49:GLN:O	1:D:51:ARG:NH1	2.16	0.79
1:E:309:THR:OG1	1:E:310:LEU:HB2	1.83	0.79
1:D:312:ARG:NH1	1:D:313:PRO:O	2.16	0.79
1:D:78:ILE:HA	1:D:81:ASN:HD21	1.47	0.79
1:A:77:SER:OG	1:A:78:ILE:N	2.13	0.78
1:E:299:VAL:HG21	1:E:313:PRO:HG3	1.64	0.78
1:B:299:VAL:HG21	1:B:313:PRO:HG3	1.65	0.78
1:E:77:SER:OG	1:E:78:ILE:N	2.09	0.78
1:E:364:GLN:HG2	1:E:377:MET:HE3	1.66	0.78
1:B:4:ARG:HG2	1:B:5:ILE:N	1.99	0.77
1:B:298:ASP:CG	1:B:299:VAL:H	1.91	0.77
1:C:291:HIS:NE2	1:C:313:PRO:HB3	1.99	0.77
1:E:306:SER:HA	1:E:309:THR:HG22	1.65	0.77
1:C:363:VAL:H	1:C:436:LYS:NZ	1.83	0.77
1:D:78:ILE:HA	1:D:81:ASN:ND2	2.00	0.77
1:B:293:GLU:OE2	1:B:298:ASP:HB2	1.85	0.77
1:D:317:ASN:OD1	1:D:318:ARG:HB2	1.85	0.77
1:A:313:PRO:HB2	1:A:316:ILE:O	1.83	0.76
1:B:344:GLY:H	1:B:349:ASN:HA	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ASP:OD2	1:C:396:VAL:HG22	1.86	0.76
1:A:297:TYR:CE1	1:A:311:PHE:HB2	2.21	0.76
1:B:466:ASN:C	1:B:467:LEU:HG	2.09	0.76
1:C:51:ARG:NH1	1:C:66:ASP:O	2.19	0.76
1:C:34:GLU:OE1	1:C:77:SER:OG	2.02	0.76
1:E:296:LYS:HG2	1:E:297:TYR:H	1.51	0.76
1:E:33:HIS:HB2	1:E:78:ILE:HG22	1.68	0.75
1:D:242:VAL:HB	1:D:310:LEU:O	1.86	0.75
1:C:51:ARG:NH1	1:C:66:ASP:OD1	2.20	0.74
1:B:466:ASN:O	1:B:467:LEU:HG	1.88	0.74
1:C:298:ASP:OD1	1:C:299:VAL:N	2.19	0.74
1:B:330:ASN:ND2	5:B:602:HOH:O	2.20	0.74
1:C:36:LEU:HB3	1:C:38:PRO:HD2	1.70	0.74
1:A:344:GLY:H	1:A:349:ASN:HA	1.53	0.74
1:A:79:LEU:HD22	1:A:84:TRP:NE1	2.03	0.73
1:A:298:ASP:HB2	1:A:300:TYR:CD1	2.23	0.73
1:B:298:ASP:OD1	1:B:299:VAL:N	2.18	0.73
1:C:8:SER:O	1:C:31:PRO:HG3	1.89	0.73
1:E:377:MET:HE1	1:E:439:ALA:HB1	1.71	0.72
1:D:6:LYS:O	5:D:601:HOH:O	2.07	0.72
1:C:393:ASP:HB2	1:C:396:VAL:N	2.05	0.71
1:A:43:VAL:HG22	1:A:72:THR:HG22	1.72	0.71
1:E:344:GLY:H	1:E:349:ASN:HA	1.56	0.71
1:A:79:LEU:HD22	1:A:84:TRP:HE1	1.56	0.71
3:C:504:EDO:O1	5:C:601:HOH:O	2.09	0.71
1:B:464:ARG:C	1:B:466:ASN:H	1.98	0.70
1:B:61:ASN:OD1	5:B:601:HOH:O	2.09	0.70
1:A:317:ASN:C	1:A:317:ASN:ND2	2.48	0.70
1:C:303:GLY:HA2	1:C:304:SER:O	1.92	0.70
1:A:56:VAL:HB	1:A:122:GLU:HG3	1.74	0.70
1:C:291:HIS:CE1	1:C:313:PRO:HB3	2.27	0.70
1:C:34:GLU:HG2	1:C:35:ALA:N	2.04	0.69
1:A:8:SER:HB3	1:A:312:ARG:HH21	1.58	0.69
1:E:297:TYR:CB	1:E:308:LYS:HD2	2.13	0.69
1:E:34:GLU:HG2	1:E:35:ALA:HB2	1.75	0.69
1:D:84:TRP:CE3	1:D:122:GLU:HA	2.28	0.69
1:B:31:PRO:HA	1:B:319:ASN:ND2	2.08	0.69
1:C:316:ILE:HG12	1:C:320:HIS:CE1	2.27	0.69
1:A:398:MET:SD	1:C:3:LYS:NZ	2.66	0.69
1:A:291:HIS:CD2	1:A:316:ILE:HG12	2.28	0.68
1:B:368:ALA:HA	1:B:369:THR:CG2	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:GLY:H	1:C:349:ASN:HA	1.57	0.68
1:B:344:GLY:N	1:B:349:ASN:HA	2.08	0.68
1:B:56:VAL:HG13	1:B:81:ASN:HB3	1.76	0.68
1:E:368:ALA:HA	1:E:369:THR:CG2	2.21	0.68
1:B:347:THR:HG21	1:B:392:TYR:HE1	1.58	0.68
1:E:30:ASP:C	1:E:318:ARG:HH22	2.02	0.68
1:B:79:LEU:HD21	1:B:84:TRP:CD1	2.25	0.68
1:A:317:ASN:H	1:A:318:ARG:HA	1.58	0.67
1:A:6:LYS:HA	1:A:33:HIS:NE2	2.09	0.67
1:A:31:PRO:HA	1:A:319:ASN:HB2	1.76	0.67
1:E:122:GLU:OE2	1:E:152:TYR:OH	2.09	0.67
1:B:323:HIS:CE1	1:B:325:LEU:HD21	2.29	0.67
1:B:293:GLU:HG3	1:B:298:ASP:CG	2.20	0.67
1:A:398:MET:HE3	1:C:3:LYS:HE3	1.76	0.67
1:B:32:GLY:N	1:B:319:ASN:HD22	1.92	0.67
1:A:184:ASP:OD1	3:A:504:EDO:H21	1.95	0.67
1:A:302:SER:HB3	1:C:309:THR:HG21	1.77	0.67
1:D:368:ALA:HA	1:D:369:THR:OG1	1.94	0.67
1:B:52:ASP:OD1	5:B:601:HOH:O	2.12	0.67
1:C:292:PHE:HB3	1:C:296:LYS:HZ2	1.60	0.66
1:C:34:GLU:OE1	1:C:78:ILE:N	2.27	0.66
1:C:318:ARG:CD	1:C:319:ASN:HB2	2.25	0.66
1:B:347:THR:HG21	1:B:392:TYR:CE1	2.31	0.66
1:B:299:VAL:HA	1:B:300:TYR:CD1	2.31	0.65
1:B:306:SER:C	1:B:308:LYS:H	2.04	0.65
1:A:422:SER:O	5:A:602:HOH:O	2.15	0.65
1:C:56:VAL:HB	1:C:122:GLU:HG3	1.77	0.65
1:A:377:MET:HE2	1:A:443:PHE:HB2	1.78	0.65
1:B:7:GLY:HA3	1:B:31:PRO:HB3	1.79	0.65
1:D:459:ASN:HA	1:D:462:LYS:HD3	1.79	0.65
1:A:316:ILE:HA	1:A:318:ARG:HG3	1.79	0.64
1:B:299:VAL:CG2	1:B:313:PRO:HG3	2.27	0.64
1:E:40:ARG:HH22	1:E:369:THR:HG21	1.62	0.64
1:B:305:GLN:HA	1:B:308:LYS:HG3	1.79	0.64
1:C:296:LYS:HG3	1:C:297:TYR:H	1.63	0.64
1:A:298:ASP:HB2	1:A:300:TYR:HD1	1.61	0.64
1:B:305:GLN:HA	1:B:308:LYS:CD	2.28	0.64
1:E:323:HIS:CE1	1:E:325:LEU:HD21	2.33	0.64
1:C:300:TYR:OH	1:C:304:SER:O	2.16	0.64
1:E:318:ARG:NH2	1:E:319:ASN:O	2.31	0.64
1:A:79:LEU:CD1	1:A:83:ILE:HA	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:HIS:NE2	1:D:77:SER:HB2	2.13	0.64
1:A:300:TYR:CG	1:A:301:GLY:N	2.67	0.63
1:A:323:HIS:CE1	1:A:325:LEU:HD21	2.33	0.63
1:E:296:LYS:HG2	1:E:297:TYR:N	2.12	0.63
1:A:298:ASP:HB3	1:A:300:TYR:HA	1.80	0.63
1:B:34:GLU:HB3	1:B:78:ILE:HD13	1.79	0.63
1:A:298:ASP:CB	1:A:300:TYR:HA	2.29	0.63
1:B:313:PRO:HB2	1:B:316:ILE:O	1.99	0.63
1:C:318:ARG:HD2	1:C:319:ASN:CB	2.27	0.63
1:D:5:ILE:O	1:D:6:LYS:HG2	1.99	0.62
1:C:307:ASP:O	1:C:308:LYS:HG3	1.99	0.62
1:E:242:VAL:HB	1:E:310:LEU:O	1.99	0.62
1:A:297:TYR:HA	1:A:308:LYS:HE3	1.81	0.62
1:B:4:ARG:HG2	1:B:5:ILE:H	1.63	0.62
1:D:49:GLN:HE21	1:D:71:TYR:HE1	1.45	0.62
1:B:323:HIS:NE2	1:B:325:LEU:HD21	2.15	0.61
1:E:433:ASN:OD1	1:E:437:LYS:NZ	2.33	0.61
1:A:466:ASN:O	1:A:467:LEU:HB3	2.00	0.61
1:A:3:LYS:N	1:B:448:LYS:HZ1	1.99	0.61
1:A:368:ALA:HA	1:A:369:THR:OG1	2.01	0.61
1:C:41:PHE:HB3	1:C:341:LEU:HD22	1.81	0.61
1:C:84:TRP:CE3	1:C:122:GLU:HA	2.36	0.61
1:D:33:HIS:CD2	1:D:77:SER:HB2	2.36	0.61
1:E:462:LYS:O	1:E:465:TYR:HB2	2.00	0.61
1:C:294:ASN:O	1:C:296:LYS:N	2.34	0.61
1:E:317:ASN:H	1:E:318:ARG:CB	2.07	0.61
1:C:300:TYR:CD2	1:C:301:GLY:N	2.69	0.60
1:A:250:TYR:CE1	1:A:292:PHE:HA	2.37	0.60
1:E:396:VAL:HA	1:E:399:ARG:HB3	1.82	0.60
1:B:347:THR:O	1:B:399:ARG:NE	2.34	0.60
1:C:43:VAL:HG22	1:C:72:THR:HG22	1.83	0.60
1:B:329:ASN:O	1:B:330:ASN:HB3	1.99	0.60
1:D:377:MET:HG2	1:D:443:PHE:HD2	1.65	0.60
1:B:75:PRO:O	1:B:76:ASN:ND2	2.34	0.60
1:B:294:ASN:O	1:B:296:LYS:N	2.31	0.60
1:C:392:TYR:O	1:C:393:ASP:HB3	2.00	0.60
1:B:29:ASN:HD21	1:B:314:ILE:HG23	1.66	0.60
1:E:56:VAL:HB	1:E:122:GLU:HG3	1.84	0.60
1:C:3:LYS:C	1:C:4:ARG:HG3	2.26	0.60
1:C:399:ARG:NH1	5:C:602:HOH:O	2.15	0.60
1:C:393:ASP:CA	1:C:395:TYR:H	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:VAL:N	1:E:300:TYR:HA	2.15	0.59
1:D:6:LYS:HZ1	1:D:153:GLU:CD	2.08	0.59
1:C:291:HIS:ND1	1:C:299:VAL:HG21	2.17	0.59
1:C:298:ASP:H	1:C:308:LYS:CE	2.13	0.59
1:E:344:GLY:N	1:E:349:ASN:HA	2.18	0.59
1:D:28:ARG:HE	1:D:323:HIS:HD1	1.48	0.59
1:D:73:SER:HB3	1:D:85:PRO:HB3	1.85	0.59
1:C:368:ALA:HA	1:C:369:THR:OG1	2.03	0.58
1:E:6:LYS:HG3	1:E:33:HIS:NE2	2.18	0.58
1:B:346:ASN:CG	1:B:347:THR:H	2.11	0.58
1:C:63:LYS:HD2	1:C:63:LYS:H	1.69	0.58
1:C:316:ILE:HG12	1:C:320:HIS:HE1	1.65	0.58
1:D:312:ARG:HH22	1:D:318:ARG:CD	2.16	0.58
1:B:301:GLY:H	1:B:305:GLN:HE22	1.51	0.58
1:B:299:VAL:HG21	1:B:313:PRO:CG	2.32	0.58
1:C:34:GLU:CG	1:C:35:ALA:H	2.07	0.58
1:A:291:HIS:HD2	1:A:316:ILE:HG12	1.69	0.58
1:B:32:GLY:H	1:B:319:ASN:HD22	1.51	0.58
1:D:56:VAL:HB	1:D:122:GLU:HG3	1.86	0.58
1:E:317:ASN:N	1:E:318:ARG:HB2	2.10	0.58
1:C:398:MET:HB2	1:D:3:LYS:HE3	1.86	0.58
1:E:359:ASN:HD21	1:E:428:GLU:HG3	1.69	0.58
1:C:292:PHE:HB3	1:C:296:LYS:NZ	2.18	0.57
1:D:75:PRO:HB3	1:D:83:ILE:HG13	1.86	0.57
1:B:242:VAL:HB	1:B:310:LEU:O	2.04	0.57
1:B:305:GLN:HA	1:B:308:LYS:CG	2.35	0.57
1:B:305:GLN:OE1	1:B:308:LYS:HB2	2.04	0.57
1:A:398:MET:CE	1:C:3:LYS:HE3	2.34	0.57
1:B:49:GLN:O	1:B:51:ARG:NH1	2.37	0.57
1:C:292:PHE:HB2	1:C:297:TYR:O	2.05	0.57
1:C:375:ASN:ND2	5:C:609:HOH:O	2.37	0.57
1:D:17:LYS:NZ	5:D:608:HOH:O	2.37	0.57
1:D:323:HIS:CE1	1:D:325:LEU:HD21	2.40	0.57
1:C:74:ILE:HG13	1:C:323:HIS:CE1	2.40	0.57
1:A:40:ARG:NH2	1:A:367:ASN:O	2.38	0.57
1:D:317:ASN:OD1	1:D:318:ARG:CB	2.52	0.57
1:A:121:GLU:HA	1:A:124:LEU:HG	1.87	0.57
1:B:29:ASN:HD21	1:B:314:ILE:HD12	1.69	0.57
1:B:34:GLU:OE2	1:B:35:ALA:HB3	2.05	0.57
1:E:29:ASN:HD21	1:E:314:ILE:HG13	1.69	0.57
1:C:304:SER:OG	1:C:307:ASP:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:HB	1:B:122:GLU:HG3	1.87	0.56
1:C:388:GLY:O	1:C:392:TYR:HA	2.04	0.56
1:B:303:GLY:H	1:B:308:LYS:NZ	2.02	0.56
1:B:316:ILE:HD12	1:B:318:ARG:HH21	1.70	0.56
1:E:79:LEU:HD11	1:E:84:TRP:NE1	2.20	0.56
1:C:40:ARG:HA	1:C:365:TYR:HD2	1.71	0.56
1:C:393:ASP:HB2	1:C:396:VAL:H	1.69	0.56
1:C:300:TYR:OH	1:C:305:GLN:HB2	2.05	0.56
1:E:73:SER:HB2	1:E:85:PRO:HB3	1.87	0.56
1:E:242:VAL:O	1:E:311:PHE:HA	2.05	0.56
1:B:43:VAL:HG22	1:B:72:THR:HG22	1.87	0.56
1:D:29:ASN:HD21	1:D:314:ILE:HG13	1.70	0.56
1:D:122:GLU:OE2	1:D:152:TYR:OH	2.23	0.56
1:D:297:TYR:OH	1:D:311:PHE:O	2.21	0.56
1:B:291:HIS:ND1	1:B:316:ILE:HG12	2.21	0.56
1:B:79:LEU:CD2	1:B:84:TRP:HD1	2.13	0.56
1:C:393:ASP:HB3	1:C:396:VAL:HG13	1.88	0.56
1:E:43:VAL:HG22	1:E:72:THR:HG22	1.86	0.56
1:D:247:ARG:HD3	1:D:314:ILE:HB	1.88	0.55
1:C:363:VAL:N	1:C:436:LYS:HZ2	1.95	0.55
1:A:31:PRO:HA	1:A:319:ASN:CB	2.35	0.55
1:A:300:TYR:OH	1:A:303:GLY:N	2.40	0.55
1:D:317:ASN:OD1	1:D:319:ASN:N	2.38	0.55
1:A:36:LEU:HD12	1:A:38:PRO:CD	2.37	0.55
1:E:459:ASN:HA	1:E:462:LYS:HD2	1.89	0.55
1:A:75:PRO:HB3	1:A:83:ILE:HG22	1.87	0.55
1:B:75:PRO:HB3	1:B:83:ILE:HG12	1.87	0.55
1:B:291:HIS:HB3	1:B:299:VAL:HB	1.88	0.55
1:C:307:ASP:C	1:C:308:LYS:HG3	2.31	0.55
1:A:40:ARG:HA	1:A:365:TYR:HD2	1.72	0.55
1:C:323:HIS:CE1	1:C:325:LEU:HD21	2.41	0.55
1:A:6:LYS:HA	1:A:33:HIS:CE1	2.42	0.54
1:B:29:ASN:ND2	1:B:314:ILE:HG23	2.22	0.54
1:D:344:GLY:H	1:D:349:ASN:HA	1.72	0.54
1:D:36:LEU:HD12	1:D:38:PRO:HD3	1.89	0.54
1:E:29:ASN:C	1:E:318:ARG:HH12	2.15	0.54
1:E:361:THR:CG2	1:E:365:TYR:HB2	2.37	0.54
1:A:6:LYS:NZ	1:A:121:GLU:OE1	2.40	0.54
1:C:393:ASP:HB2	1:C:395:TYR:N	2.23	0.54
1:B:34:GLU:HB3	1:B:78:ILE:CD1	2.38	0.54
1:D:295:THR:HG22	1:D:296:LYS:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:462:LYS:O	1:D:465:TYR:CZ	2.60	0.54
1:D:153:GLU:OE2	5:D:603:HOH:O	2.19	0.54
1:C:73:SER:O	1:C:74:ILE:HD13	2.07	0.54
1:C:242:VAL:HG12	1:C:311:PHE:HE1	1.73	0.54
1:C:344:GLY:N	1:C:349:ASN:HA	2.23	0.54
1:A:292:PHE:HB2	1:A:297:TYR:HD2	1.72	0.53
1:E:299:VAL:HA	1:E:300:TYR:HB3	1.89	0.53
1:D:295:THR:HG22	1:D:296:LYS:HG2	1.90	0.53
1:D:312:ARG:HG3	1:D:312:ARG:HH11	1.73	0.53
1:B:361:THR:HG23	1:B:362:PRO:HD2	1.90	0.53
1:C:316:ILE:CG1	1:C:320:HIS:HE1	2.21	0.53
1:A:323:HIS:NE2	1:A:325:LEU:HD21	2.23	0.53
1:E:79:LEU:HD11	1:E:84:TRP:HE1	1.73	0.53
1:B:297:TYR:CD1	1:B:307:ASP:O	2.62	0.53
1:D:28:ARG:NH1	1:D:30:ASP:HB2	2.24	0.53
1:D:78:ILE:O	1:D:79:LEU:HD23	2.09	0.53
1:E:250:TYR:CE1	1:E:292:PHE:HA	2.43	0.53
1:D:45:ASN:ND2	5:D:611:HOH:O	2.41	0.53
1:E:394:PHE:CZ	1:E:456:THR:HG22	2.44	0.53
1:A:325:LEU:HD22	1:A:339:HIS:HD2	1.74	0.52
1:B:51:ARG:HD3	5:B:649:HOH:O	2.09	0.52
1:C:323:HIS:NE2	1:C:325:LEU:HD21	2.24	0.52
1:A:333:THR:HG23	5:A:718:HOH:O	2.09	0.52
1:B:462:LYS:HG3	1:B:463:LEU:HD12	1.90	0.52
1:D:289:SER:C	1:D:315:GLY:H	2.17	0.52
1:E:33:HIS:CB	1:E:78:ILE:HG22	2.39	0.52
1:A:317:ASN:N	1:A:318:ARG:HA	2.23	0.52
1:C:291:HIS:NE2	1:C:316:ILE:HB	2.23	0.52
1:C:412:LYS:HE3	1:C:416:ASP:OD2	2.08	0.52
1:E:79:LEU:HD12	1:E:81:ASN:OD1	2.09	0.52
1:E:396:VAL:HG13	1:E:399:ARG:HD3	1.92	0.52
1:B:29:ASN:ND2	1:B:314:ILE:HD12	2.24	0.52
1:C:34:GLU:HB3	1:C:77:SER:OG	2.10	0.52
1:A:8:SER:HB2	1:A:243:TYR:OH	2.09	0.52
1:B:304:SER:C	1:B:308:LYS:HD2	2.35	0.52
1:A:304:SER:OG	1:A:305:GLN:N	2.43	0.51
1:B:39:GLN:NE2	1:B:40:ARG:O	2.43	0.51
1:C:464:ARG:CA	1:C:466:ASN:H	2.22	0.51
1:D:41:PHE:HB3	1:D:341:LEU:HD22	1.92	0.51
1:D:296:LYS:O	1:D:304:SER:HB3	2.09	0.51
1:B:79:LEU:HD13	1:B:82:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:LYS:CG	1:B:463:LEU:HD12	2.40	0.51
1:A:34:GLU:CD	1:A:35:ALA:H	2.18	0.51
1:A:324:ILE:HB	1:A:340:TRP:HB2	1.92	0.51
1:B:325:LEU:HD22	1:B:339:HIS:CD2	2.45	0.51
1:A:297:TYR:HA	1:A:308:LYS:CE	2.41	0.51
1:B:465:TYR:HD2	1:B:466:ASN:C	2.19	0.51
1:C:469:ASP:C	1:C:469:ASP:OD1	2.53	0.51
1:D:73:SER:O	1:D:74:ILE:HD13	2.11	0.51
1:B:293:GLU:OE1	1:B:294:ASN:HA	2.10	0.51
1:C:363:VAL:HG13	1:C:436:LYS:HZ1	1.75	0.51
1:B:51:ARG:NE	1:B:66:ASP:OD1	2.41	0.51
1:D:315:GLY:O	1:D:320:HIS:ND1	2.44	0.51
1:E:324:ILE:HB	1:E:340:TRP:HB2	1.92	0.51
1:A:300:TYR:CD1	1:A:308:LYS:HD3	2.46	0.51
1:C:192:ARG:O	1:C:194:ASN:ND2	2.43	0.51
1:C:464:ARG:HA	1:C:466:ASN:H	1.76	0.51
1:B:348:PHE:HA	1:B:399:ARG:CZ	2.40	0.51
1:B:464:ARG:C	1:B:466:ASN:N	2.63	0.51
1:C:300:TYR:CD1	1:C:308:LYS:HD2	2.45	0.51
1:E:40:ARG:HG3	1:E:365:TYR:HB3	1.93	0.51
1:B:291:HIS:CE1	1:B:316:ILE:HD11	2.47	0.51
1:D:242:VAL:HG11	1:D:310:LEU:HD13	1.93	0.51
1:A:6:LYS:HE2	1:A:101:THR:OG1	2.12	0.50
1:B:250:TYR:CE1	1:B:292:PHE:HA	2.46	0.50
1:C:72:THR:OG1	1:C:339:HIS:NE2	2.37	0.50
1:B:84:TRP:CE3	1:B:122:GLU:HA	2.46	0.50
1:C:393:ASP:HA	1:C:395:TYR:H	1.76	0.50
1:D:37:ASP:OD2	1:D:345:ALA:HB2	2.11	0.50
1:A:377:MET:HG2	1:A:443:PHE:HD1	1.75	0.50
1:A:344:GLY:N	1:A:349:ASN:HA	2.22	0.50
1:B:320:HIS:CE1	1:B:349:ASN:HD21	2.28	0.50
1:A:78:ILE:C	1:A:79:LEU:HG	2.33	0.50
1:B:6:LYS:NZ	1:B:153:GLU:OE2	2.36	0.50
1:D:212:LYS:NZ	1:D:216:ASP:OD2	2.44	0.50
1:A:41:PHE:HB3	1:A:341:LEU:HD22	1.94	0.50
1:A:361:THR:HG23	1:A:362:PRO:HD2	1.94	0.50
1:E:192:ARG:O	1:E:194:ASN:ND2	2.45	0.50
1:E:300:TYR:CE1	1:E:305:GLN:CD	2.90	0.50
1:E:320:HIS:N	1:E:320:HIS:CD2	2.79	0.50
1:A:67:ASP:OD1	1:A:67:ASP:N	2.45	0.50
1:A:291:HIS:HB3	1:A:316:ILE:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLU:CD	1:C:78:ILE:HB	2.36	0.50
1:B:3:LYS:HG3	1:B:4:ARG:H	1.76	0.50
1:E:8:SER:HB2	1:E:312:ARG:HH12	1.76	0.50
1:E:296:LYS:HZ3	1:E:297:TYR:HD2	1.58	0.50
1:A:13:LEU:HB3	1:A:165:VAL:HG11	1.94	0.50
1:B:139:VAL:HG13	1:B:168:LEU:HD12	1.94	0.50
1:D:250:TYR:CE1	1:D:292:PHE:HA	2.47	0.50
1:E:461:MET:O	1:E:464:ARG:HG2	2.11	0.50
1:A:346:ASN:CG	1:A:347:THR:H	2.19	0.49
1:C:291:HIS:ND1	1:C:299:VAL:CG2	2.75	0.49
1:E:41:PHE:HB3	1:E:341:LEU:HD22	1.94	0.49
1:B:31:PRO:HA	1:B:319:ASN:HD22	1.77	0.49
1:C:259:ASP:OD2	3:C:504:EDO:H11	2.11	0.49
1:E:359:ASN:HD22	1:E:359:ASN:H	1.53	0.49
1:A:49:GLN:O	1:A:51:ARG:NH1	2.45	0.49
1:A:291:HIS:HD2	1:A:316:ILE:HG21	1.78	0.49
1:A:78:ILE:HD12	1:A:79:LEU:H	1.77	0.49
1:B:28:ARG:HD3	1:B:97:SER:OG	2.12	0.49
1:D:28:ARG:HD3	1:D:97:SER:OG	2.13	0.49
1:D:303:GLY:HA3	1:E:306:SER:OG	2.12	0.49
1:E:465:TYR:CZ	1:E:467:LEU:O	2.65	0.49
1:B:51:ARG:HD2	1:B:66:ASP:HA	1.94	0.49
1:E:86:ALA:HB1	1:E:99:THR:CG2	2.43	0.49
1:E:6:LYS:NZ	1:E:121:GLU:OE2	2.45	0.49
1:E:346:ASN:HB2	1:E:385:ALA:HB1	1.95	0.49
1:B:298:ASP:CG	1:B:299:VAL:N	2.64	0.49
1:D:5:ILE:HD12	1:D:5:ILE:H	1.78	0.49
1:D:324:ILE:HB	1:D:340:TRP:HB2	1.96	0.48
1:E:136:ARG:O	1:E:140:LYS:HG3	2.12	0.48
1:E:318:ARG:HD2	1:E:319:ASN:N	2.21	0.48
1:E:463:LEU:HA	1:E:465:TYR:CB	2.43	0.48
1:B:299:VAL:HG11	1:B:313:PRO:HG3	1.94	0.48
1:B:299:VAL:CG1	1:B:313:PRO:HG3	2.43	0.48
1:E:74:ILE:HD13	1:E:323:HIS:CE1	2.48	0.48
1:A:325:LEU:HD22	1:A:339:HIS:CD2	2.48	0.48
1:E:299:VAL:HA	1:E:300:TYR:CB	2.42	0.48
1:E:398:MET:HE2	1:E:449:LEU:HD12	1.95	0.48
1:A:399:ARG:NH2	1:A:403:GLU:OE1	2.46	0.48
1:B:4:ARG:HG2	1:B:5:ILE:HG12	1.96	0.48
1:B:5:ILE:O	1:B:6:LYS:HB2	2.12	0.48
1:D:315:GLY:HA3	1:D:320:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:PHE:HB3	1:E:296:LYS:NZ	2.29	0.48
1:E:323:HIS:NE2	1:E:325:LEU:HD21	2.29	0.48
1:A:274:HIS:NE2	3:A:504:EDO:H11	2.28	0.48
1:A:318:ARG:CD	1:A:320:HIS:HB2	2.43	0.48
1:B:307:ASP:C	1:B:308:LYS:HG2	2.39	0.48
1:C:299:VAL:HG23	1:C:299:VAL:O	2.12	0.48
1:C:37:ASP:N	1:C:38:PRO:CD	2.76	0.48
1:C:291:HIS:CD2	1:C:314:ILE:H	2.32	0.48
1:D:291:HIS:HB2	1:D:313:PRO:HB3	1.95	0.48
1:E:76:ASN:HB3	1:E:77:SER:H	1.47	0.48
1:A:212:LYS:NZ	1:A:216:ASP:OD2	2.45	0.48
1:B:313:PRO:CB	1:B:316:ILE:HB	2.44	0.48
1:D:152:TYR:CE1	1:D:153:GLU:HG3	2.50	0.47
1:B:30:ASP:CB	1:B:321:ASN:HB2	2.41	0.47
1:E:359:ASN:N	1:E:428:GLU:OE2	2.40	0.47
1:A:392:TYR:O	1:A:396:VAL:HG23	2.14	0.47
1:B:297:TYR:CE1	1:B:307:ASP:O	2.67	0.47
1:C:8:SER:HB2	1:C:243:TYR:OH	2.14	0.47
1:C:392:TYR:O	1:C:392:TYR:CG	2.67	0.47
1:C:464:ARG:C	1:C:466:ASN:N	2.72	0.47
1:D:317:ASN:ND2	1:D:320:HIS:HA	2.30	0.47
1:A:333:THR:HG22	5:A:722:HOH:O	2.15	0.47
1:C:76:ASN:ND2	1:C:84:TRP:CH2	2.83	0.47
1:C:291:HIS:CD2	1:C:316:ILE:HG13	2.50	0.47
1:C:335:ILE:HG22	1:C:431:LEU:HD21	1.96	0.47
1:A:292:PHE:HB2	1:A:297:TYR:CD2	2.50	0.47
1:E:28:ARG:HD3	1:E:97:SER:OG	2.15	0.47
1:E:139:VAL:HG13	1:E:168:LEU:HD12	1.95	0.47
1:A:412:LYS:HE3	1:A:416:ASP:OD2	2.15	0.47
1:B:38:PRO:HB3	1:B:378:TYR:CD1	2.49	0.47
1:C:291:HIS:CD2	1:C:314:ILE:N	2.82	0.47
1:E:319:ASN:N	1:E:319:ASN:OD1	2.47	0.47
1:A:86:ALA:HB1	1:A:99:THR:CG2	2.45	0.47
1:D:72:THR:OG1	1:D:339:HIS:HE1	1.97	0.47
1:D:312:ARG:HH22	1:D:318:ARG:HD3	1.78	0.47
1:D:380:LEU:HG	1:D:446:GLN:HG3	1.96	0.47
1:E:361:THR:HG23	1:E:362:PRO:HD2	1.97	0.47
1:A:79:LEU:HD13	1:A:83:ILE:HA	1.96	0.47
1:A:113:PRO:HD2	5:A:687:HOH:O	2.15	0.47
1:B:67:ASP:OD1	1:B:67:ASP:N	2.47	0.47
1:C:28:ARG:HD2	1:C:99:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ASP:HB3	1:C:378:TYR:HE1	1.80	0.47
1:C:40:ARG:HA	1:C:365:TYR:CD2	2.50	0.47
1:B:30:ASP:O	1:B:319:ASN:ND2	2.48	0.47
1:B:71:TYR:CE1	1:B:130:PRO:HG3	2.50	0.47
1:C:5:ILE:O	1:C:6:LYS:HG2	2.15	0.47
1:D:317:ASN:OD1	1:D:319:ASN:C	2.58	0.47
1:A:136:ARG:NE	5:A:605:HOH:O	2.37	0.46
1:B:72:THR:OG1	1:B:339:HIS:HE1	1.98	0.46
1:C:28:ARG:HD3	1:C:97:SER:OG	2.15	0.46
1:D:293:GLU:O	1:D:293:GLU:HG2	2.15	0.46
1:A:72:THR:OG1	1:A:339:HIS:HE1	1.99	0.46
1:C:464:ARG:C	1:C:466:ASN:H	2.21	0.46
1:D:36:LEU:HD12	1:D:38:PRO:CD	2.45	0.46
1:C:300:TYR:CE1	1:C:308:LYS:HD2	2.50	0.46
1:B:5:ILE:HG22	1:B:6:LYS:N	2.31	0.46
1:A:51:ARG:HD2	1:A:66:ASP:HA	1.96	0.46
1:B:346:ASN:CG	1:B:347:THR:N	2.74	0.46
1:B:335:ILE:HG22	1:B:431:LEU:HD11	1.98	0.46
1:C:398:MET:HE3	1:D:3:LYS:CE	2.45	0.46
1:D:139:VAL:HG13	1:D:168:LEU:HD12	1.97	0.46
1:E:67:ASP:OD1	1:E:67:ASP:N	2.48	0.46
1:E:359:ASN:N	1:E:359:ASN:ND2	2.50	0.46
1:A:32:GLY:H	1:A:319:ASN:CG	2.24	0.46
1:B:78:ILE:C	1:B:79:LEU:HD12	2.41	0.46
1:C:74:ILE:HG13	1:C:323:HIS:NE2	2.30	0.46
1:D:315:GLY:O	1:D:317:ASN:HB2	2.16	0.46
1:A:300:TYR:CD2	1:A:301:GLY:N	2.84	0.46
1:A:300:TYR:CZ	1:A:304:SER:O	2.69	0.46
1:E:359:ASN:ND2	1:E:428:GLU:HG3	2.31	0.46
1:B:39:GLN:NE2	1:B:74:ILE:HG23	2.31	0.46
1:B:289:SER:OG	1:B:320:HIS:NE2	2.48	0.46
1:B:5:ILE:H	1:B:5:ILE:HD13	1.81	0.46
1:B:8:SER:O	1:B:31:PRO:HD3	2.16	0.46
1:B:262:ASP:O	1:B:264:PRO:HD3	2.16	0.46
1:B:303:GLY:N	1:B:308:LYS:NZ	2.64	0.46
1:B:312:ARG:HA	1:B:313:PRO:HD2	1.39	0.46
1:D:86:ALA:HB1	1:D:99:THR:CG2	2.46	0.46
1:E:8:SER:N	1:E:31:PRO:HG2	2.31	0.46
1:A:152:TYR:CE1	1:A:153:GLU:HG3	2.51	0.45
1:C:207:CYS:HB2	1:C:211:LEU:HD22	1.97	0.45
1:C:324:ILE:HB	1:C:340:TRP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ASP:CG	1:C:396:VAL:HG13	2.41	0.45
1:D:437:LYS:NZ	5:D:618:HOH:O	2.45	0.45
1:B:301:GLY:H	1:B:305:GLN:NE2	2.15	0.45
1:B:320:HIS:CD2	1:B:322:VAL:HG23	2.51	0.45
1:C:393:ASP:CB	1:C:396:VAL:HG13	2.46	0.45
1:D:323:HIS:NE2	1:D:325:LEU:HD21	2.31	0.45
1:E:364:GLN:CG	1:E:377:MET:HE3	2.43	0.45
1:A:361:THR:HG21	1:A:365:TYR:HB2	1.97	0.45
1:B:314:ILE:HA	1:B:315:GLY:HA2	1.60	0.45
1:C:363:VAL:HG22	1:C:436:LYS:NZ	2.31	0.45
1:E:398:MET:HE1	1:E:452:ASP:HB2	1.98	0.45
1:A:433:ASN:OD1	1:A:437:LYS:NZ	2.48	0.45
1:E:239:LYS:HD2	1:E:239:LYS:HA	1.84	0.45
1:A:308:LYS:O	1:A:309:THR:OG1	2.33	0.45
1:A:344:GLY:HA2	1:A:345:ALA:HA	1.78	0.45
1:C:465:TYR:OH	1:C:468:ASN:OD1	2.18	0.45
1:B:4:ARG:CG	1:B:5:ILE:N	2.77	0.45
1:C:307:ASP:O	1:C:308:LYS:CG	2.65	0.45
1:C:318:ARG:HH21	1:C:319:ASN:N	2.14	0.45
1:D:43:VAL:HG22	1:D:72:THR:HG22	1.99	0.45
1:D:315:GLY:HA3	1:D:320:HIS:HE1	1.82	0.45
1:E:152:TYR:CE2	1:E:153:GLU:HG3	2.51	0.45
1:B:458:SER:O	1:B:462:LYS:HB3	2.17	0.45
1:D:29:ASN:HA	1:D:321:ASN:O	2.17	0.45
1:D:312:ARG:HA	1:D:313:PRO:HD2	1.80	0.45
1:D:361:THR:CG2	1:D:365:TYR:HB2	2.47	0.45
1:A:318:ARG:HH22	1:A:347:THR:HG22	1.82	0.44
1:A:298:ASP:HB2	1:A:300:TYR:HA	1.99	0.44
1:B:28:ARG:HE	1:B:323:HIS:HD1	1.65	0.44
1:B:362:PRO:HB2	1:B:364:GLN:HG2	1.99	0.44
1:E:314:ILE:HA	1:E:315:GLY:HA2	1.58	0.44
1:A:335:ILE:HG22	1:A:431:LEU:HD21	1.99	0.44
1:D:426:ASP:OD2	1:D:429:LYS:HD3	2.17	0.44
1:E:10:THR:OG1	1:E:314:ILE:HG12	2.18	0.44
1:A:247:ARG:HG2	1:A:314:ILE:HG12	1.99	0.44
1:C:291:HIS:HE2	1:C:313:PRO:HB3	1.80	0.44
1:E:361:THR:HG22	1:E:365:TYR:HB2	2.00	0.44
1:E:376:ASN:OD1	1:E:378:TYR:HB3	2.17	0.44
1:A:8:SER:CB	1:A:312:ARG:HH21	2.27	0.44
1:C:291:HIS:O	1:C:292:PHE:HB2	2.17	0.44
1:E:39:GLN:CD	1:E:39:GLN:H	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ARG:HD2	1:E:66:ASP:HA	2.00	0.44
1:A:305:GLN:HA	1:A:308:LYS:HB2	1.99	0.44
1:A:314:ILE:HA	1:A:315:GLY:HA2	1.66	0.44
1:B:132:VAL:HG11	1:B:138:GLY:HA2	1.99	0.44
1:B:316:ILE:HD12	1:B:318:ARG:NH2	2.32	0.44
1:B:317:ASN:OD1	1:B:319:ASN:OD1	2.36	0.44
1:B:319:ASN:O	1:B:319:ASN:CG	2.61	0.44
1:A:10:THR:OG1	1:A:314:ILE:HG21	2.18	0.44
1:A:305:GLN:O	1:A:305:GLN:HG2	2.18	0.44
1:A:411:ARG:HH11	3:A:503:EDO:H21	1.83	0.44
1:B:324:ILE:HB	1:B:340:TRP:HB2	1.99	0.44
1:E:374:LEU:HA	1:E:374:LEU:HD23	1.78	0.44
1:E:412:LYS:HE3	1:E:416:ASP:OD2	2.18	0.44
1:A:312:ARG:HA	1:A:313:PRO:HD2	1.59	0.44
1:B:299:VAL:HA	1:B:300:TYR:CG	2.53	0.44
1:B:347:THR:O	1:B:399:ARG:CZ	2.65	0.44
1:C:300:TYR:CE1	1:C:305:GLN:HG3	2.52	0.44
1:C:393:ASP:HB2	1:C:395:TYR:H	1.81	0.44
1:A:8:SER:O	1:A:31:PRO:HD3	2.18	0.43
1:B:399:ARG:HH11	1:B:402:TYR:HD2	1.66	0.43
1:C:197:GLN:CD	1:C:197:GLN:H	2.26	0.43
1:B:306:SER:C	1:B:308:LYS:N	2.73	0.43
1:C:286:PHE:HZ	1:D:238:ILE:HD11	1.82	0.43
1:D:293:GLU:N	1:D:293:GLU:OE1	2.51	0.43
1:E:309:THR:OG1	1:E:310:LEU:N	2.51	0.43
1:E:398:MET:HE1	1:E:452:ASP:CB	2.47	0.43
1:B:344:GLY:HA2	1:B:345:ALA:HA	1.79	0.43
1:B:465:TYR:HD2	1:B:466:ASN:O	2.01	0.43
1:C:139:VAL:HG13	1:C:168:LEU:HD12	2.00	0.43
1:A:293:GLU:O	1:A:293:GLU:HG2	2.18	0.43
1:A:300:TYR:OH	1:A:304:SER:O	2.34	0.43
1:D:76:ASN:ND2	1:D:86:ALA:HB2	2.33	0.43
1:C:393:ASP:CB	1:C:396:VAL:N	2.80	0.43
1:D:71:TYR:CE1	1:D:130:PRO:HG3	2.54	0.43
1:D:332:PRO:HD2	1:D:335:ILE:HD11	1.99	0.43
1:E:71:TYR:CE1	1:E:130:PRO:HG3	2.52	0.43
1:B:298:ASP:C	1:B:300:TYR:HA	2.43	0.43
1:A:398:MET:HE3	1:A:398:MET:HB2	1.91	0.43
1:B:249:TRP:CZ2	1:B:253:LYS:HG3	2.53	0.43
1:D:374:LEU:HA	1:D:374:LEU:HD23	1.74	0.43
1:E:392:TYR:CD1	1:E:392:TYR:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLU:HG2	5:A:628:HOH:O	2.19	0.43
1:E:242:VAL:HA	1:E:311:PHE:CD1	2.54	0.43
1:B:239:LYS:HE2	1:B:243:TYR:CG	2.54	0.43
1:B:361:THR:HG21	1:B:365:TYR:HB2	2.00	0.43
1:D:122:GLU:CD	1:D:122:GLU:H	2.26	0.43
1:D:317:ASN:ND2	1:D:318:ARG:NH2	2.67	0.43
1:D:343:TYR:HA	1:D:344:GLY:HA3	1.84	0.43
1:D:398:MET:HE3	1:E:3:LYS:HD3	2.00	0.43
1:D:465:TYR:CD1	1:D:465:TYR:N	2.81	0.43
1:A:84:TRP:CE3	1:A:122:GLU:HA	2.54	0.43
1:C:32:GLY:O	1:C:318:ARG:NH2	2.50	0.43
1:C:361:THR:CG2	1:C:365:TYR:HB2	2.49	0.43
1:D:291:HIS:ND1	1:D:316:ILE:HG12	2.34	0.43
1:D:361:THR:HG23	1:D:362:PRO:HD2	2.00	0.43
1:C:202:SER:O	5:C:603:HOH:O	2.22	0.42
1:A:5:ILE:HG23	1:A:33:HIS:CD2	2.54	0.42
1:A:346:ASN:HB2	1:A:385:ALA:HB1	2.00	0.42
1:C:59:LYS:NZ	5:C:622:HOH:O	2.52	0.42
1:D:83:ILE:HG23	1:D:83:ILE:O	2.19	0.42
1:B:4:ARG:CG	1:B:5:ILE:HG12	2.49	0.42
1:D:314:ILE:HA	1:D:315:GLY:HA2	1.62	0.42
1:E:298:ASP:C	1:E:300:TYR:HA	2.43	0.42
1:A:32:GLY:H	1:A:319:ASN:CB	2.32	0.42
1:A:249:TRP:CZ2	1:A:253:LYS:HG3	2.54	0.42
1:D:242:VAL:HG12	1:D:311:PHE:HE1	1.85	0.42
1:A:6:LYS:HD2	1:A:121:GLU:OE2	2.20	0.42
1:A:292:PHE:HB2	1:A:297:TYR:O	2.20	0.42
1:B:34:GLU:CD	1:B:35:ALA:HB3	2.44	0.42
1:C:78:ILE:O	1:C:79:LEU:HD12	2.18	0.42
1:C:200:PHE:CD2	1:C:212:LYS:HD2	2.54	0.42
1:A:393:ASP:HA	1:A:396:VAL:HG23	2.01	0.42
1:A:398:MET:SD	1:C:3:LYS:CE	3.08	0.42
1:A:463:LEU:HA	1:A:465:TYR:O	2.19	0.42
1:C:376:ASN:OD1	1:C:378:TYR:HB3	2.20	0.42
1:E:296:LYS:CG	1:E:297:TYR:N	2.77	0.42
1:B:72:THR:OG1	1:B:339:HIS:CE1	2.73	0.42
1:B:291:HIS:ND1	1:B:316:ILE:CG1	2.82	0.42
1:B:313:PRO:HB2	1:B:316:ILE:HB	2.00	0.42
1:C:296:LYS:HG3	1:C:297:TYR:N	2.33	0.42
1:C:317:ASN:HA	1:C:318:ARG:HA	1.40	0.42
1:A:318:ARG:HH22	1:A:347:THR:CG2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:LEU:HD22	1:B:339:HIS:HD2	1.83	0.42
1:B:361:THR:CG2	1:B:365:TYR:HB2	2.50	0.42
1:B:398:MET:HE3	1:B:398:MET:HB2	1.93	0.42
1:B:399:ARG:NH1	1:B:402:TYR:CD2	2.88	0.42
1:C:198:PHE:HB2	1:C:229:LEU:HG	2.02	0.42
1:E:300:TYR:HE1	1:E:305:GLN:NE2	2.18	0.42
1:E:312:ARG:HA	1:E:313:PRO:HD2	1.72	0.42
5:A:604:HOH:O	1:C:3:LYS:N	2.52	0.42
1:B:84:TRP:CD2	1:B:122:GLU:HA	2.54	0.42
1:D:454:VAL:O	1:D:458:SER:HB3	2.20	0.42
1:E:362:PRO:HB2	1:E:365:TYR:HD1	1.84	0.42
1:A:361:THR:CG2	1:A:365:TYR:HB2	2.50	0.41
1:D:462:LYS:O	1:D:464:ARG:N	2.53	0.41
1:E:30:ASP:HB3	1:E:321:ASN:HB2	2.00	0.41
1:E:344:GLY:HA2	1:E:345:ALA:HA	1.77	0.41
1:B:303:GLY:HA2	1:B:304:SER:HA	1.76	0.41
1:C:86:ALA:HB1	1:C:99:THR:CG2	2.50	0.41
1:E:34:GLU:HG2	1:E:35:ALA:N	2.35	0.41
1:B:299:VAL:O	1:B:299:VAL:HG12	2.19	0.41
1:C:73:SER:OG	1:C:85:PRO:HB3	2.19	0.41
1:D:313:PRO:HB2	1:D:316:ILE:O	2.21	0.41
1:E:34:GLU:HG2	1:E:35:ALA:CB	2.48	0.41
1:B:376:ASN:OD1	1:B:378:TYR:HB3	2.20	0.41
1:D:376:ASN:OD1	1:D:378:TYR:HB3	2.20	0.41
1:E:398:MET:HE3	1:E:398:MET:HB2	1.82	0.41
1:C:291:HIS:CD2	1:C:316:ILE:H	2.39	0.41
1:C:394:PHE:CE1	1:C:460:ASN:ND2	2.89	0.41
1:E:84:TRP:CE3	1:E:122:GLU:HA	2.55	0.41
1:A:299:VAL:O	1:A:299:VAL:HG12	2.20	0.41
1:A:346:ASN:CG	1:A:347:THR:N	2.79	0.41
1:D:412:LYS:NZ	5:D:613:HOH:O	2.43	0.41
1:C:250:TYR:CE1	1:C:292:PHE:HA	2.56	0.41
1:C:312:ARG:HA	1:C:313:PRO:HD2	1.30	0.41
1:C:393:ASP:HB2	1:C:395:TYR:C	2.45	0.41
1:C:13:LEU:HB3	1:C:165:VAL:HG11	2.03	0.41
1:C:132:VAL:HG11	1:C:138:GLY:HA2	2.02	0.41
1:C:374:LEU:HA	1:C:374:LEU:HD23	1.78	0.41
1:D:29:ASN:ND2	1:D:314:ILE:HG13	2.36	0.41
1:D:344:GLY:N	1:D:349:ASN:HA	2.35	0.41
1:B:83:ILE:O	1:B:83:ILE:HG23	2.21	0.41
1:B:305:GLN:HA	1:B:308:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:TYR:HA	1:B:344:GLY:HA3	1.84	0.41
1:C:30:ASP:HB3	1:C:321:ASN:HB2	2.03	0.41
1:C:462:LYS:HE3	1:C:462:LYS:HB2	1.70	0.41
1:D:8:SER:N	1:D:31:PRO:HG3	2.36	0.41
1:D:446:GLN:OE1	1:D:449:LEU:HD23	2.21	0.41
1:E:40:ARG:HD2	1:E:365:TYR:HA	2.02	0.41
1:E:347:THR:HG21	1:E:392:TYR:CE1	2.56	0.41
1:E:465:TYR:OH	1:E:468:ASN:HA	2.21	0.41
1:B:4:ARG:CG	1:B:5:ILE:H	2.30	0.41
1:B:4:ARG:NH1	1:B:57:ILE:HG21	2.35	0.41
1:C:74:ILE:CG1	1:C:323:HIS:CE1	3.03	0.41
1:C:441:VAL:O	1:C:445:LYS:HB2	2.21	0.41
1:D:312:ARG:HH22	1:D:318:ARG:HD2	1.85	0.41
1:E:8:SER:HB2	1:E:243:TYR:OH	2.21	0.41
1:E:220:LEU:HD23	1:E:220:LEU:HA	1.91	0.41
1:E:458:SER:O	1:E:462:LYS:HD2	2.21	0.41
1:A:343:TYR:HA	1:A:344:GLY:HA3	1.89	0.40
1:C:291:HIS:NE2	1:C:313:PRO:CB	2.77	0.40
1:E:78:ILE:HD12	1:E:78:ILE:HA	1.95	0.40
1:E:317:ASN:N	1:E:318:ARG:CB	2.79	0.40
1:A:3:LYS:HE2	1:B:398:MET:HA	2.02	0.40
1:A:262:ASP:O	1:A:264:PRO:HD3	2.22	0.40
1:A:295:THR:CG2	1:C:310:LEU:HD21	2.51	0.40
1:B:299:VAL:N	1:B:300:TYR:HA	2.36	0.40
1:D:152:TYR:CD1	1:D:153:GLU:HG3	2.55	0.40
1:D:309:THR:HB	1:D:310:LEU:H	1.70	0.40
1:D:462:LYS:HG3	1:D:465:TYR:OH	2.21	0.40
1:A:51:ARG:HD3	5:A:639:HOH:O	2.20	0.40
1:A:86:ALA:HB1	1:A:99:THR:HG21	2.03	0.40
1:D:13:LEU:HB3	1:D:165:VAL:HG11	2.03	0.40
1:E:362:PRO:HD3	5:E:653:HOH:O	2.22	0.40
1:A:57:ILE:HD13	1:A:80:THR:HG22	2.04	0.40
1:B:297:TYR:HD1	1:B:307:ASP:O	2.03	0.40
1:B:433:ASN:OD1	1:B:437:LYS:NZ	2.55	0.40
1:C:316:ILE:CG1	1:C:320:HIS:CE1	3.00	0.40
1:D:72:THR:OG1	1:D:339:HIS:CE1	2.74	0.40
1:B:291:HIS:O	1:B:292:PHE:HB2	2.22	0.40
1:B:465:TYR:C	1:B:465:TYR:CD2	3.00	0.40
1:E:296:LYS:HZ2	1:E:297:TYR:HB2	1.86	0.40
1:E:393:ASP:HA	1:E:396:VAL:HG23	2.04	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	465/469 (99%)	418 (90%)	41 (9%)	6 (1%)	9	16
1	B	465/469 (99%)	410 (88%)	46 (10%)	9 (2%)	6	10
1	C	465/469 (99%)	414 (89%)	40 (9%)	11 (2%)	4	7
1	D	465/469 (99%)	416 (90%)	44 (10%)	5 (1%)	11	20
1	E	465/469 (99%)	410 (88%)	48 (10%)	7 (2%)	8	14
All	All	2325/2345 (99%)	2068 (89%)	219 (9%)	38 (2%)	7	13

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	77	SER
1	A	468	ASN
1	B	5	ILE
1	B	6	LYS
1	B	295	THR
1	B	465	TYR
1	C	295	THR
1	C	304	SER
1	C	309	THR
1	C	317	ASN
1	C	468	ASN
1	D	295	THR
1	E	296	LYS
1	E	304	SER
1	E	305	GLN
1	A	296	LYS
1	A	309	THR
1	B	35	ALA
1	B	319	ASN
1	B	468	ASN

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Mol	Chain	Res	Type
1	C	465	TYR
1	D	318	ARG
1	A	467	LEU
1	C	305	GLN
1	E	34	GLU
1	D	79	LEU
1	E	467	LEU
1	B	467	LEU
1	C	292	PHE
1	C	313	PRO
1	E	292	PHE
1	C	37	ASP
1	C	75	PRO
1	B	83	ILE
1	E	75	PRO
1	D	83	ILE
1	D	190	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	413/415 (100%)	397 (96%)	16 (4%)	28	52
1	B	413/415 (100%)	403 (98%)	10 (2%)	43	67
1	C	413/415 (100%)	404 (98%)	9 (2%)	45	70
1	D	413/415 (100%)	404 (98%)	9 (2%)	45	70
1	E	413/415 (100%)	396 (96%)	17 (4%)	27	50
All	All	2065/2075 (100%)	2004 (97%)	61 (3%)	36	61

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	79	LEU

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Mol	Chain	Res	Type
1	A	80	THR
1	A	295	THR
1	A	308	LYS
1	A	314	ILE
1	A	316	ILE
1	A	317	ASN
1	A	319	ASN
1	A	339	HIS
1	A	361	THR
1	A	366	LYS
1	A	384	THR
1	A	396	VAL
1	A	446	GLN
1	A	463	LEU
1	B	5	ILE
1	B	291	HIS
1	B	295	THR
1	B	308	LYS
1	B	312	ARG
1	B	314	ILE
1	B	316	ILE
1	B	361	THR
1	B	396	VAL
1	B	446	GLN
1	C	36	LEU
1	C	83	ILE
1	C	291	HIS
1	C	314	ILE
1	C	320	HIS
1	C	393	ASP
1	C	399	ARG
1	C	462	LYS
1	C	469	ASP
1	D	3	LYS
1	D	5	ILE
1	D	33	HIS
1	D	122	GLU
1	D	308	LYS
1	D	316	ILE
1	D	339	HIS
1	D	396	VAL
1	D	467	LEU

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Mol	Chain	Res	Type
1	E	36	LEU
1	E	40	ARG
1	E	47	GLU
1	E	51	ARG
1	E	73	SER
1	E	78	ILE
1	E	122	GLU
1	E	187	VAL
1	E	299	VAL
1	E	316	ILE
1	E	319	ASN
1	E	320	HIS
1	E	359	ASN
1	E	384	THR
1	E	393	ASP
1	E	425	LYS
1	E	459	ASN

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

Mol	Chain	Res	Type
1	A	61	ASN
1	A	162	ASN
1	A	252	GLN
1	A	291	HIS
1	A	294	ASN
1	A	317	ASN
1	A	339	HIS
1	A	367	ASN
1	B	33	HIS
1	B	61	ASN
1	B	76	ASN
1	B	319	ASN
1	B	330	ASN
1	B	339	HIS
1	B	447	ASN
1	C	81	ASN
1	C	162	ASN
1	C	320	HIS
1	D	339	HIS
1	D	367	ASN
1	D	447	ASN

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Mol	Chain	Res	Type
1	D	460	ASN
1	E	162	ASN
1	E	305	GLN
1	E	359	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACT	B	502	-	3,3,3	0.82	0	3,3,3	1.67	2 (66%)
3	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.31	0
3	EDO	A	505	-	3,3,3	0.68	0	2,2,2	0.30	0
3	EDO	A	503	-	3,3,3	0.46	0	2,2,2	0.21	0
3	EDO	C	503	-	3,3,3	0.54	0	2,2,2	0.22	0
3	EDO	C	504	-	3,3,3	0.71	0	2,2,2	0.24	0

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
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	A	503	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	502	ACT	OXT-C-O	-2.07	114.35	122.03
4	B	502	ACT	OXT-C-CH3	2.03	123.56	115.05

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	504	EDO	O1-C1-C2-O2
3	A	503	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	504	EDO	2	0
3	A	503	EDO	1	0
3	C	504	EDO	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

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	467/469 (99%)	0.16	55 (11%) 9 7	21, 35, 100, 125	0
1	B	467/469 (99%)	0.28	60 (12%) 7 6	24, 38, 108, 130	0
1	C	467/469 (99%)	0.34	61 (13%) 7 6	25, 42, 106, 128	0
1	D	467/469 (99%)	0.42	61 (13%) 7 6	29, 45, 109, 129	0
1	E	467/469 (99%)	0.40	60 (12%) 7 6	27, 45, 105, 131	0
All	All	2335/2345 (99%)	0.32	297 (12%) 8 6	21, 42, 106, 131	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	LEU	6.6
1	A	315	GLY	6.2
1	E	32	GLY	6.2
1	D	32	GLY	6.0
1	D	467	LEU	5.9
1	B	32	GLY	5.8
1	C	299	VAL	5.6
1	A	316	ILE	5.5
1	C	467	LEU	5.5
1	A	468	ASN	5.4
1	A	314	ILE	5.3
1	B	37	ASP	5.3
1	E	316	ILE	5.2
1	D	368	ALA	5.2
1	D	310	LEU	5.2
1	D	31	PRO	5.2
1	C	314	ILE	5.2
1	B	309	THR	5.0
1	A	310	LEU	5.0
1	C	33	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	79	LEU	4.9
1	E	310	LEU	4.9
1	C	310	LEU	4.9
1	E	314	ILE	4.8
1	D	469	ASP	4.8
1	A	31	PRO	4.7
1	B	314	ILE	4.7
1	C	316	ILE	4.6
1	D	314	ILE	4.6
1	A	463	LEU	4.6
1	B	368	ALA	4.6
1	B	5	ILE	4.6
1	C	5	ILE	4.6
1	C	468	ASN	4.6
1	E	467	LEU	4.5
1	E	83	ILE	4.5
1	C	79	LEU	4.5
1	E	35	ALA	4.4
1	E	315	GLY	4.4
1	D	309	THR	4.3
1	E	80	THR	4.3
1	B	468	ASN	4.3
1	B	467	LEU	4.3
1	B	313	PRO	4.3
1	B	81	ASN	4.2
1	D	316	ILE	4.2
1	E	311	PHE	4.2
1	E	297	TYR	4.2
1	E	299	VAL	4.2
1	C	35	ALA	4.2
1	A	297	TYR	4.1
1	D	299	VAL	4.1
1	D	465	TYR	4.1
1	C	312	ARG	4.1
1	C	469	ASP	4.1
1	B	297	TYR	4.1
1	E	392	TYR	4.1
1	A	292	PHE	4.1
1	C	344	GLY	4.1
1	A	32	GLY	4.0
1	C	77	SER	4.0
1	D	300	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	33	HIS	4.0
1	B	33	HIS	4.0
1	E	31	PRO	4.0
1	D	468	ASN	3.9
1	C	82	GLY	3.9
1	E	36	LEU	3.9
1	B	76	ASN	3.9
1	C	319	ASN	3.9
1	B	315	GLY	3.9
1	D	5	ILE	3.9
1	A	469	ASP	3.9
1	C	297	TYR	3.8
1	C	3	LYS	3.8
1	A	299	VAL	3.8
1	C	294	ASN	3.8
1	E	82	GLY	3.8
1	E	313	PRO	3.8
1	C	315	GLY	3.8
1	B	463	LEU	3.8
1	D	78	ILE	3.8
1	B	39	GLN	3.7
1	D	80	THR	3.7
1	B	36	LEU	3.7
1	E	81	ASN	3.7
1	B	31	PRO	3.7
1	C	313	PRO	3.7
1	D	293	GLU	3.7
1	A	294	ASN	3.7
1	A	37	ASP	3.7
1	A	313	PRO	3.7
1	E	33	HIS	3.7
1	D	311	PHE	3.7
1	D	33	HIS	3.6
1	C	32	GLY	3.6
1	D	315	GLY	3.6
1	D	344	GLY	3.6
1	B	82	GLY	3.6
1	D	463	LEU	3.6
1	B	312	ARG	3.6
1	A	293	GLU	3.6
1	E	312	ARG	3.6
1	B	294	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	34	GLU	3.6
1	A	78	ILE	3.6
1	C	295	THR	3.5
1	C	309	THR	3.5
1	D	82	GLY	3.5
1	E	295	THR	3.5
1	D	292	PHE	3.5
1	A	392	TYR	3.5
1	B	300	TYR	3.5
1	C	465	TYR	3.5
1	E	78	ILE	3.5
1	E	292	PHE	3.5
1	E	463	LEU	3.4
1	D	313	PRO	3.4
1	A	467	LEU	3.4
1	A	82	GLY	3.4
1	A	344	GLY	3.4
1	B	83	ILE	3.4
1	B	316	ILE	3.4
1	B	465	TYR	3.4
1	A	368	ALA	3.4
1	B	292	PHE	3.4
1	E	461	MET	3.4
1	E	390	THR	3.3
1	E	320	HIS	3.3
1	D	304	SER	3.3
1	A	76	ASN	3.3
1	C	81	ASN	3.3
1	E	294	ASN	3.3
1	D	312	ARG	3.3
1	C	300	TYR	3.3
1	C	393	ASP	3.3
1	E	465	TYR	3.3
1	A	36	LEU	3.3
1	D	35	ALA	3.3
1	B	392	TYR	3.3
1	D	36	LEU	3.3
1	E	344	GLY	3.3
1	E	469	ASP	3.2
1	A	295	THR	3.2
1	C	311	PHE	3.2
1	B	3	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	76	ASN	3.2
1	D	319	ASN	3.2
1	D	297	TYR	3.2
1	E	300	TYR	3.2
1	B	80	THR	3.2
1	D	76	ASN	3.2
1	E	396	VAL	3.1
1	C	293	GLU	3.1
1	A	77	SER	3.1
1	C	463	LEU	3.1
1	A	35	ALA	3.1
1	B	319	ASN	3.1
1	D	301	GLY	3.1
1	C	392	TYR	3.0
1	A	79	LEU	3.0
1	D	294	ASN	3.0
1	B	469	ASP	3.0
1	C	40	ARG	3.0
1	B	311	PHE	3.0
1	B	348	PHE	3.0
1	E	5	ILE	3.0
1	A	34	GLU	3.0
1	D	295	THR	3.0
1	D	77	SER	3.0
1	D	81	ASN	3.0
1	C	78	ILE	2.9
1	C	317	ASN	2.9
1	D	460	ASN	2.9
1	D	461	MET	2.9
1	D	37	ASP	2.9
1	B	344	GLY	2.9
1	B	461	MET	2.9
1	A	291	HIS	2.9
1	C	6	LYS	2.9
1	A	81	ASN	2.9
1	C	395	TYR	2.9
1	A	465	TYR	2.8
1	C	301	GLY	2.8
1	A	319	ASN	2.8
1	B	302	SER	2.8
1	C	396	VAL	2.8
1	A	300	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	299	VAL	2.8
1	B	35	ALA	2.8
1	C	36	LEU	2.8
1	C	296	LYS	2.8
1	A	304	SER	2.8
1	B	330	ASN	2.8
1	A	312	ARG	2.8
1	C	37	ASP	2.8
1	C	302	SER	2.7
1	D	345	ALA	2.7
1	E	37	ASP	2.7
1	B	343	TYR	2.7
1	D	302	SER	2.7
1	D	83	ILE	2.7
1	D	318	ARG	2.7
1	A	320	HIS	2.7
1	D	291	HIS	2.7
1	E	291	HIS	2.7
1	B	393	ASP	2.6
1	B	293	GLU	2.6
1	E	293	GLU	2.6
1	A	80	THR	2.6
1	B	361	THR	2.6
1	E	368	ALA	2.6
1	D	306	SER	2.6
1	A	309	THR	2.6
1	A	345	ALA	2.6
1	B	295	THR	2.6
1	E	395	TYR	2.6
1	A	4	ARG	2.6
1	B	464	ARG	2.6
1	C	318	ARG	2.6
1	B	78	ILE	2.6
1	B	77	SER	2.6
1	C	323	HIS	2.6
1	B	369	THR	2.5
1	D	369	THR	2.5
1	E	307	ASP	2.5
1	C	345	ALA	2.5
1	D	4	ARG	2.5
1	E	298	ASP	2.5
1	C	292	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	303	GLY	2.4
1	D	34	GLU	2.4
1	D	392	TYR	2.4
1	C	291	HIS	2.4
1	A	398	MET	2.4
1	D	390	THR	2.4
1	E	77	SER	2.4
1	D	3	LYS	2.4
1	A	5	ILE	2.4
1	C	4	ARG	2.4
1	B	318	ARG	2.4
1	D	320	HIS	2.4
1	E	4	ARG	2.4
1	B	303	GLY	2.4
1	B	291	HIS	2.4
1	A	318	ARG	2.3
1	D	308	LYS	2.3
1	B	460	ASN	2.3
1	E	317	ASN	2.3
1	D	464	ARG	2.3
1	A	30	ASP	2.3
1	E	242	VAL	2.3
1	E	34	GLU	2.3
1	B	40	ARG	2.3
1	C	99	THR	2.3
1	E	42	VAL	2.3
1	B	320	HIS	2.2
1	E	423	GLY	2.2
1	A	83	ILE	2.2
1	C	304	SER	2.2
1	D	307	ASP	2.2
1	A	369	THR	2.2
1	B	364	GLN	2.2
1	C	320	HIS	2.2
1	A	7	GLY	2.2
1	D	296	LYS	2.2
1	B	345	ALA	2.2
1	E	321	ASN	2.2
1	E	468	ASN	2.2
1	C	80	THR	2.2
1	D	303	GLY	2.2
1	B	30	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	6	LYS	2.2
1	B	363	VAL	2.1
1	C	330	ASN	2.1
1	D	321	ASN	2.1
1	C	369	THR	2.1
1	E	302	SER	2.1
1	C	308	LYS	2.1
1	A	311	PHE	2.1
1	D	39	GLN	2.1
1	E	76	ASN	2.1
1	E	466	ASN	2.1
1	E	3	LYS	2.1
1	E	359	ASN	2.1
1	C	83	ILE	2.1
1	A	296	LYS	2.1
1	C	368	ALA	2.1
1	E	345	ALA	2.1
1	E	464	ARG	2.1
1	A	390	THR	2.1
1	A	38	PRO	2.1
1	E	303	GLY	2.0
1	C	298	ASP	2.0
1	A	461	MET	2.0
1	E	43	VAL	2.0
1	A	466	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	EDO	A	504	4/4	0.62	0.18	37,37,42,42	0
3	EDO	C	504	4/4	0.78	0.17	37,41,46,46	0
4	ACT	B	502	4/4	0.82	0.21	33,46,47,47	0
3	EDO	A	505	4/4	0.84	0.15	30,34,38,43	0
2	CO	A	501	1/1	0.88	0.26	85,85,85,85	0
3	EDO	C	503	4/4	0.88	0.11	36,39,39,44	0
2	CO	D	501	1/1	0.89	0.11	91,91,91,91	0
2	CO	C	501	1/1	0.90	0.11	90,90,90,90	0
2	CO	B	501	1/1	0.93	0.06	81,81,81,81	0
2	CO	C	502	1/1	0.93	0.07	70,70,70,70	0
3	EDO	A	503	4/4	0.98	0.07	29,32,35,35	0
2	CO	A	502	1/1	0.99	0.04	50,50,50,50	0
2	CO	E	501	1/1	0.99	0.13	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.