



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:11 AM UTC

PDB ID : 4P2V / pdb_00004p2v
Title : Structure of the AI-2 processing enzyme LsrF in complex with the product of the LsrG reaction P-HPD
Authors : Miller, S.T.; Oh, I.K.; Xavier, K.B.
Deposited on : 2014-03-04
Resolution : 2.51 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

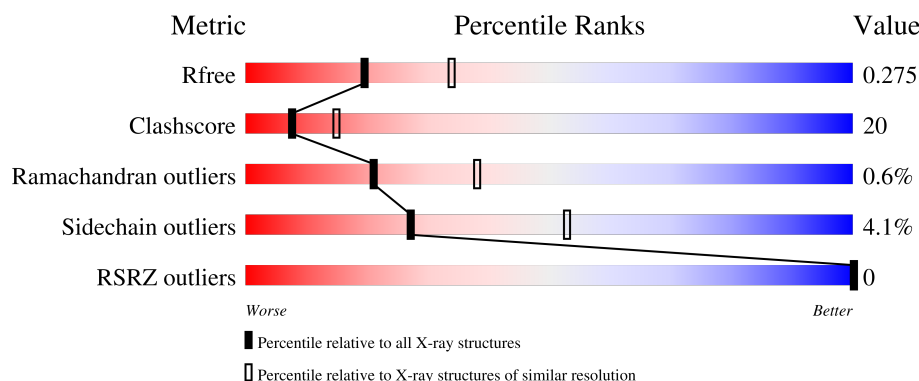
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	293	
1	B	293	
1	C	293	
1	D	293	
1	E	293	

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Mol	Chain	Length	Quality of chain
1	F	293	 71% 23% . .
1	G	293	 55% 34% 5% . .
1	H	293	 56% 37% . . .
1	I	293	 60% 32% . . .
1	K	293	 60% 32% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22178 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 Uncharacterized aldolase LsrF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	B	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	C	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	D	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	E	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	F	280	Total	C	N	O	S	0	0	0
			2138	1345	377	398	18			
1	G	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	H	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	I	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	K	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			

There are 30 discrepancies between the modelled and reference sequences:

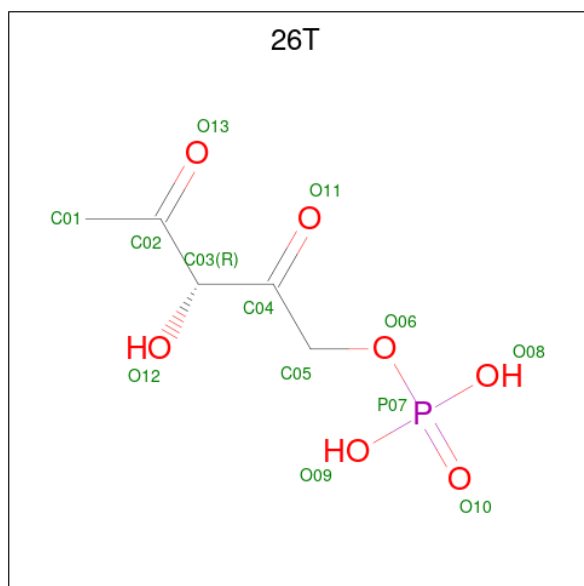
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P76143
A	0	SER	-	expression tag	UNP P76143
A	203	ALA	LYS	engineered mutation	UNP P76143
B	-1	GLY	-	expression tag	UNP P76143
B	0	SER	-	expression tag	UNP P76143
B	203	ALA	LYS	engineered mutation	UNP P76143
C	-1	GLY	-	expression tag	UNP P76143
C	0	SER	-	expression tag	UNP P76143
C	203	ALA	LYS	engineered mutation	UNP P76143

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P76143
D	0	SER	-	expression tag	UNP P76143
D	203	ALA	LYS	engineered mutation	UNP P76143
E	-1	GLY	-	expression tag	UNP P76143
E	0	SER	-	expression tag	UNP P76143
E	203	ALA	LYS	engineered mutation	UNP P76143
F	-1	GLY	-	expression tag	UNP P76143
F	0	SER	-	expression tag	UNP P76143
F	203	ALA	LYS	engineered mutation	UNP P76143
G	-1	GLY	-	expression tag	UNP P76143
G	0	SER	-	expression tag	UNP P76143
G	203	ALA	LYS	engineered mutation	UNP P76143
H	-1	GLY	-	expression tag	UNP P76143
H	0	SER	-	expression tag	UNP P76143
H	203	ALA	LYS	engineered mutation	UNP P76143
I	-1	GLY	-	expression tag	UNP P76143
I	0	SER	-	expression tag	UNP P76143
I	203	ALA	LYS	engineered mutation	UNP P76143
K	-1	GLY	-	expression tag	UNP P76143
K	0	SER	-	expression tag	UNP P76143
K	203	ALA	LYS	engineered mutation	UNP P76143

- Molecule 2 is (3R)-3-hydroxy-2,4-dioxopentyl dihydrogen phosphate (CCD ID: 26T) (formula: C₅H₉O₇P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O P 13 5 7 1	0	0
2	B	1	Total C O P 13 5 7 1	0	0
2	C	1	Total C O P 13 5 7 1	0	0
2	D	1	Total C O P 13 5 7 1	0	0
2	E	1	Total C O P 13 5 7 1	0	0
2	F	1	Total C O P 13 5 7 1	0	0
2	G	1	Total C O P 13 5 7 1	0	0
2	H	1	Total C O P 13 5 7 1	0	0
2	I	1	Total C O P 13 5 7 1	0	0
2	K	1	Total C O P 13 5 7 1	0	0

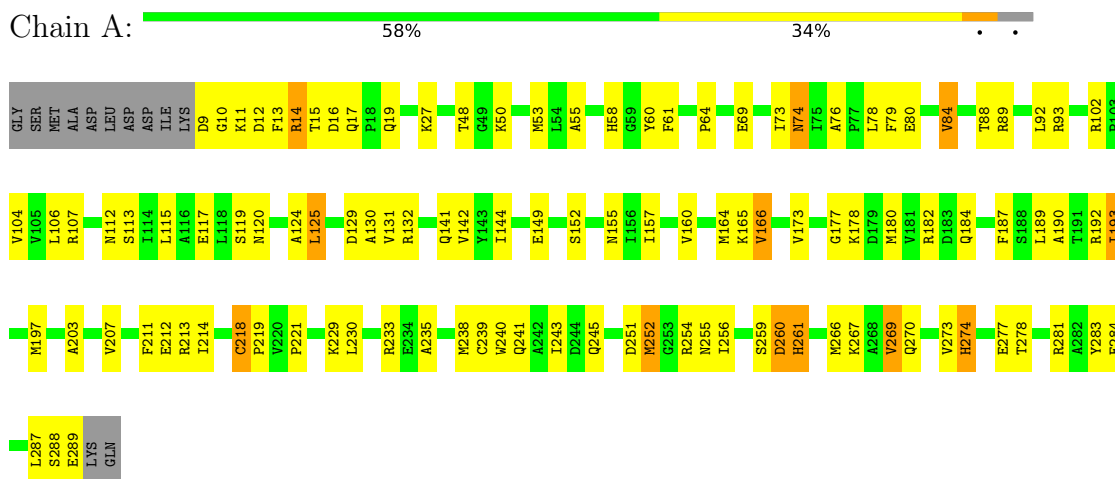
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	47	Total O 47 47	0	0
3	B	73	Total O 73 73	0	0
3	C	66	Total O 66 66	0	0
3	D	38	Total O 38 38	0	0
3	E	71	Total O 71 71	0	0
3	F	85	Total O 85 85	0	0
3	G	47	Total O 47 47	0	0
3	H	47	Total O 47 47	0	0
3	I	80	Total O 80 80	0	0
3	K	42	Total O 42 42	0	0

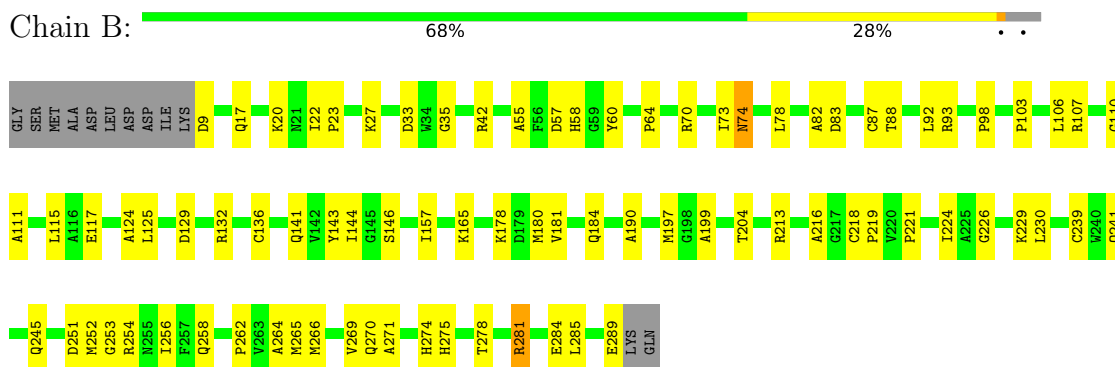
3 Residue-property plots

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.

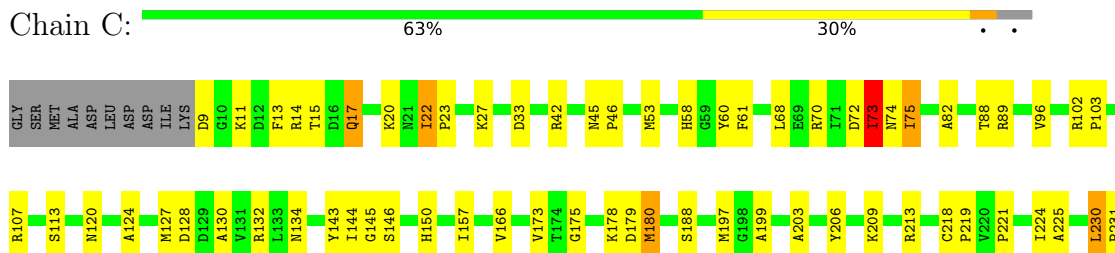
• Molecule 1: Uncharacterized aldolase LsrF



• Molecule 1: Uncharacterized aldolase LsrF



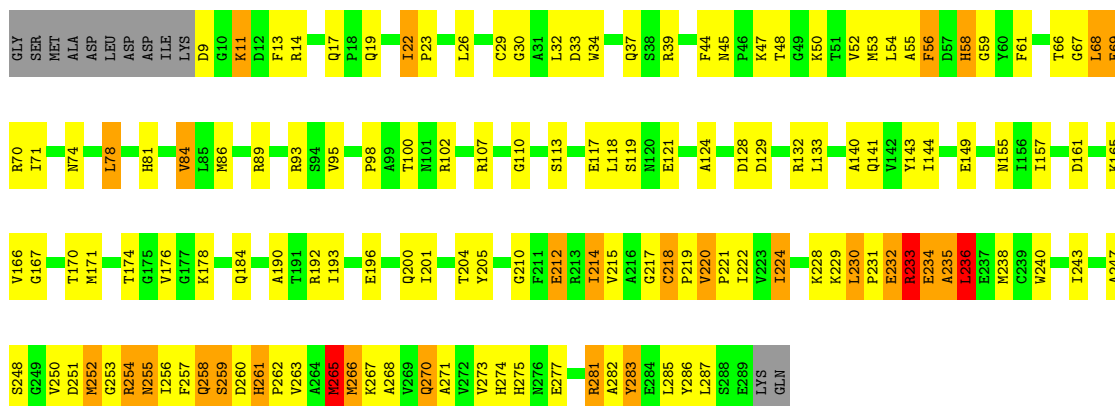
• Molecule 1: Uncharacterized aldolase LsrF





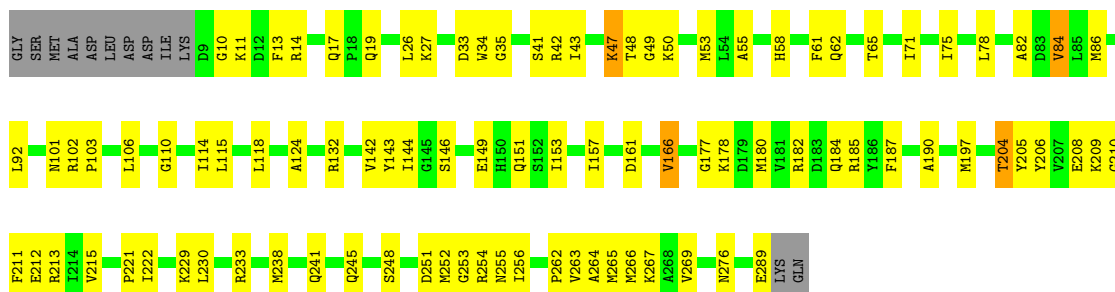
• Molecule 1: Uncharacterized aldolase LsrF

Chain D: 49% 37% 9% . .



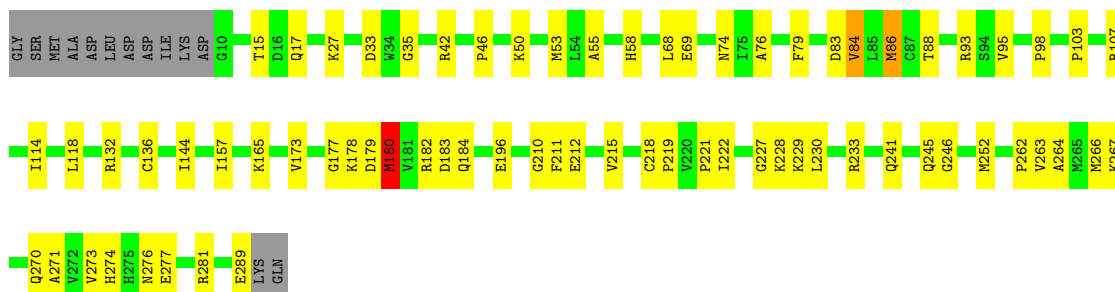
• Molecule 1: Uncharacterized aldolase LsrF

Chain E: 64% 31% . .



• Molecule 1: Uncharacterized aldolase LsrF

Chain F: 71% 23% . .



• Molecule 1: Uncharacterized aldolase LsrF

Chain G: 55% 34% 5% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.62Å 105.74Å 170.40Å 90.00° 101.43° 90.00°	Depositor
Resolution (Å)	49.26 – 2.51 49.26 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.26-2.51) 90.0 (49.26-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1626)	Depositor
R, R_{free}	0.235 , 0.271 0.236 , 0.275	Depositor DCC
R_{free} test set	4585 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22178	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 3.49% 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: 26T

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	0.48	0/2185	1.04	7/2957 (0.2%)
1	B	0.37	0/2185	0.91	2/2957 (0.1%)
1	C	0.44	0/2185	1.05	13/2957 (0.4%)
1	D	0.61	2/2185 (0.1%)	1.20	21/2957 (0.7%)
1	E	0.38	0/2185	0.89	1/2957 (0.0%)
1	F	0.40	1/2177 (0.0%)	0.88	2/2946 (0.1%)
1	G	0.48	0/2185	1.15	16/2957 (0.5%)
1	H	0.49	0/2185	1.05	10/2957 (0.3%)
1	I	0.57	1/2185 (0.0%)	1.02	7/2957 (0.2%)
1	K	0.43	0/2185	1.06	7/2957 (0.2%)
All	All	0.47	4/21842 (0.0%)	1.03	86/29559 (0.3%)

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	G	0	4
1	I	0	1
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	185	ARG	C-N	17.26	1.58	1.33
1	D	234	GLU	CA-C	-9.94	1.48	1.53
1	F	180	MET	C-N	7.97	1.41	1.33
1	D	258	GLN	C-N	6.34	1.42	1.33

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	73	ILE	N-CA-C	13.44	122.24	111.62
1	D	232	GLU	N-CA-C	11.15	126.02	111.75
1	D	236	LEU	N-CA-C	-10.93	99.95	113.18
1	G	281	ARG	N-CA-C	-9.94	100.83	113.16
1	G	260	ASP	N-CA-C	-9.31	101.62	113.16
1	K	256	ILE	CB-CA-C	-8.40	104.57	111.71
1	G	81	HIS	N-CA-C	8.20	124.28	113.30
1	H	279	ALA	N-CA-C	7.94	119.57	111.07
1	D	230	LEU	N-CA-C	-7.93	98.45	110.50
1	K	119	SER	N-CA-C	-7.20	104.50	113.28
1	C	180	MET	N-CA-C	7.04	120.72	109.24
1	K	287	LEU	CA-CB-CG	-6.95	91.98	116.30
1	D	232	GLU	CA-C-N	-6.90	112.40	123.23
1	D	232	GLU	C-N-CA	-6.90	112.40	123.23
1	G	274	HIS	N-CA-C	6.86	118.84	111.36
1	G	184	GLN	CA-CB-CG	6.72	127.53	114.10
1	A	261	HIS	CA-C-N	6.66	126.45	119.05
1	A	261	HIS	C-N-CA	6.66	126.45	119.05
1	I	282	ALA	N-CA-C	-6.54	103.99	112.23
1	C	241	GLN	CA-CB-CG	-6.46	101.19	114.10
1	G	176	VAL	N-CA-C	6.28	119.04	109.12
1	D	218	CYS	CA-C-N	6.26	126.38	119.87
1	D	218	CYS	C-N-CA	6.26	126.38	119.87
1	C	281	ARG	N-CA-C	-6.23	105.62	113.72
1	C	73	ILE	N-CA-CB	-6.18	106.57	111.64
1	H	281	ARG	N-CA-C	-6.14	105.82	113.38
1	D	267	LYS	N-CA-C	-6.14	104.65	111.71
1	D	234	GLU	CA-C-O	6.08	122.16	118.33
1	I	80	GLU	CA-C-N	-6.05	112.97	122.65
1	I	80	GLU	C-N-CA	-6.05	112.97	122.65
1	E	10	GLY	N-CA-C	-5.99	105.33	115.34
1	D	259	SER	N-CA-C	-5.97	102.47	110.24
1	H	80	GLU	CA-C-N	-5.96	113.14	122.73
1	H	80	GLU	C-N-CA	-5.96	113.14	122.73
1	D	265	MET	N-CA-C	5.89	117.79	111.36
1	D	68	LEU	N-CA-C	-5.89	105.41	112.59
1	G	79	PHE	N-CA-C	-5.86	104.23	111.33
1	H	181	VAL	CA-C-N	5.84	132.22	121.70
1	H	181	VAL	C-N-CA	5.84	132.22	121.70
1	A	10	GLY	N-CA-C	-5.73	99.61	113.18
1	F	17	GLN	CA-C-N	5.71	125.66	119.78
1	F	17	GLN	C-N-CA	5.71	125.66	119.78
1	I	177	GLY	N-CA-C	5.70	126.69	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	10	GLY	N-CA-C	-5.68	106.20	115.46
1	D	22	ILE	CA-C-N	5.67	125.60	119.76
1	D	22	ILE	C-N-CA	5.67	125.60	119.76
1	H	246	GLY	N-CA-C	5.62	122.87	114.95
1	K	261	HIS	CA-C-N	5.59	125.26	119.05
1	K	261	HIS	C-N-CA	5.59	125.26	119.05
1	D	261	HIS	CA-C-N	5.57	125.23	119.05
1	D	261	HIS	C-N-CA	5.57	125.23	119.05
1	I	249	GLY	N-CA-C	5.57	117.50	110.38
1	C	230	LEU	CA-C-N	-5.55	114.04	119.76
1	C	230	LEU	C-N-CA	-5.55	114.04	119.76
1	G	286	TYR	CA-CB-CG	5.54	123.88	113.90
1	D	234	GLU	CB-CA-C	-5.54	108.38	116.53
1	I	281	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	H	284	GLU	N-CA-C	-5.45	106.48	113.01
1	G	180	MET	CA-C-N	-5.42	114.31	122.01
1	G	180	MET	C-N-CA	-5.42	114.31	122.01
1	C	75	ILE	N-CA-C	-5.42	107.08	113.42
1	A	74	ASN	N-CA-CB	-5.37	103.20	110.67
1	C	22	ILE	CA-C-N	5.33	125.25	119.76
1	C	22	ILE	C-N-CA	5.33	125.25	119.76
1	A	218	CYS	CA-C-N	5.33	125.41	119.87
1	A	218	CYS	C-N-CA	5.33	125.41	119.87
1	B	181	VAL	N-CA-C	5.30	115.84	108.84
1	G	76	ALA	CA-C-N	-5.28	114.26	120.12
1	G	76	ALA	C-N-CA	-5.28	114.26	120.12
1	I	280	ASP	N-CA-C	-5.28	106.52	113.17
1	C	96	VAL	N-CA-C	5.27	112.77	107.55
1	G	285	LEU	N-CA-C	-5.24	106.74	112.72
1	G	183	ASP	CA-C-N	5.19	127.23	120.28
1	G	183	ASP	C-N-CA	5.19	127.23	120.28
1	K	246	GLY	N-CA-C	5.19	122.26	114.95
1	D	230	LEU	CB-CA-C	5.16	116.81	108.91
1	H	235	ALA	N-CA-C	5.16	117.81	111.82
1	A	252	MET	N-CA-C	5.10	116.62	108.41
1	H	67	GLY	N-CA-C	-5.09	108.63	114.69
1	G	287	LEU	N-CA-C	5.07	121.60	110.80
1	B	281	ARG	N-CA-C	-5.07	107.27	113.50
1	D	233	ARG	CA-C-N	-5.03	117.74	123.13
1	D	233	ARG	C-N-CA	-5.03	117.74	123.13
1	C	17	GLN	CA-C-N	5.01	124.94	119.78
1	C	17	GLN	C-N-CA	5.01	124.94	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	281	ARG	N-CA-C	-5.01	106.42	112.88

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	280	ASP	Peptide
1	G	285	LEU	Peptide
1	G	286	TYR	Peptide
1	G	287	LEU	Peptide
1	I	178	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2146	0	2148	101	0
1	B	2146	0	2148	67	0
1	C	2146	0	2148	83	1
1	D	2146	0	2148	181	1
1	E	2146	0	2148	74	0
1	F	2138	0	2144	54	0
1	G	2146	0	2148	116	0
1	H	2146	0	2148	106	0
1	I	2146	0	2148	91	0
1	K	2146	0	2148	91	0
2	A	13	0	9	1	0
2	B	13	0	9	3	0
2	C	13	0	9	0	0
2	D	13	0	9	4	0
2	E	13	0	9	2	0
2	F	13	0	9	1	0
2	G	13	0	9	2	0
2	H	13	0	9	3	0
2	I	13	0	9	3	0
2	K	13	0	9	1	0
3	A	47	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	73	0	0	14	0
3	C	66	0	0	10	1
3	D	38	0	0	13	0
3	E	71	0	0	17	0
3	F	85	0	0	10	0
3	G	47	0	0	17	0
3	H	47	0	0	14	0
3	I	80	0	0	15	1
3	K	42	0	0	6	0
All	All	22178	0	21566	867	2

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 20.

All (867) 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:D:256:ILE:HG23	1:D:265:MET:SD	1.30	1.64
1:D:256:ILE:CG2	1:D:265:MET:SD	2.20	1.30
1:G:278:THR:OG1	1:G:281:ARG:CG	1.92	1.18
1:G:278:THR:OG1	1:G:281:ARG:HG2	0.99	1.15
1:A:78:LEU:HB3	1:A:266:MET:HE1	1.36	1.07
1:B:281:ARG:NH1	3:B:402:HOH:O	1.91	1.01
1:D:23:PRO:O	3:D:416:HOH:O	1.82	0.97
1:A:141:GLN:O	3:A:413:HOH:O	1.81	0.96
1:G:268:ALA:HA	1:G:285:LEU:HD12	1.48	0.96
1:H:234:GLU:O	3:H:441:HOH:O	1.83	0.95
1:D:256:ILE:HG12	1:D:265:MET:HE1	1.48	0.95
1:D:252:MET:HE2	1:D:265:MET:HE1	1.48	0.92
1:H:181:VAL:HA	1:H:182:ARG:HB2	1.52	0.92
1:D:254:ARG:HA	1:D:257:PHE:CE1	2.05	0.92
1:I:176:VAL:HG22	1:I:178:LYS:HD3	1.50	0.91
1:H:23:PRO:O	3:H:403:HOH:O	1.86	0.91
1:G:278:THR:HG1	1:G:281:ARG:HG2	1.10	0.90
1:G:169:PRO:HA	1:G:200:GLN:HE21	1.36	0.90
1:G:84:VAL:HG12	1:G:103:PRO:HB2	1.50	0.90
1:B:74:ASN:H	1:B:74:ASN:HD22	1.18	0.90
1:F:196:GLU:OE2	3:F:415:HOH:O	1.88	0.89
1:G:43:ILE:HG22	1:G:84:VAL:HG11	1.55	0.89
1:D:220:VAL:HG12	1:D:221:PRO:HD2	1.55	0.88
1:B:60:TYR:O	3:B:409:HOH:O	1.91	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:ALA:O	1:G:282:ALA:HB3	1.74	0.87
1:D:66:THR:OG1	1:D:258:GLN:NE2	2.07	0.86
1:E:75:ILE:HD12	1:E:78:LEU:HD12	1.57	0.85
1:F:276:ASN:OD1	3:F:468:HOH:O	1.93	0.85
1:B:74:ASN:HD22	1:B:74:ASN:N	1.75	0.85
1:G:82:ALA:O	1:G:102:ARG:NH2	2.10	0.85
1:E:177:GLY:H	1:E:180:MET:HE3	1.42	0.84
1:G:48:THR:HB	1:G:50:LYS:HE3	1.57	0.84
1:C:23:PRO:O	3:C:416:HOH:O	1.95	0.84
1:D:229:LYS:HA	1:D:255:ASN:HD22	1.43	0.84
1:G:230:LEU:HD12	1:G:231:PRO:HD2	1.60	0.83
1:D:59:GLY:O	3:D:402:HOH:O	1.95	0.83
1:K:226:GLY:O	3:K:424:HOH:O	1.96	0.83
1:G:276:ASN:HA	3:G:419:HOH:O	1.79	0.83
1:D:256:ILE:CG1	1:D:265:MET:HE1	2.09	0.82
1:D:256:ILE:HG12	1:D:265:MET:CE	2.10	0.82
1:D:174:THR:HG21	1:D:190:ALA:HB1	1.62	0.82
1:D:265:MET:HG3	1:D:266:MET:N	1.95	0.81
1:D:256:ILE:CD1	1:D:265:MET:HE1	2.10	0.81
1:A:89:ARG:HD3	1:A:125:LEU:HD12	1.63	0.80
1:A:164:MET:SD	1:D:93:ARG:NH1	2.53	0.80
1:G:147:GLU:O	3:G:406:HOH:O	1.99	0.80
1:H:236:LEU:HD11	1:H:268:ALA:HB1	1.64	0.80
1:D:19:GLN:OE1	1:G:70:ARG:NH2	2.15	0.79
1:I:74:ASN:N	1:I:74:ASN:HD22	1.80	0.79
1:D:233:ARG:HD3	1:D:283:TYR:HB2	1.62	0.79
1:D:30:GLY:O	3:D:410:HOH:O	2.01	0.79
1:H:229:LYS:NZ	1:H:230:LEU:O	2.16	0.79
1:H:51:THR:O	3:H:443:HOH:O	1.99	0.79
1:I:80:GLU:HG3	1:I:81:HIS:ND1	1.98	0.79
1:E:161:ASP:OD2	3:E:449:HOH:O	2.00	0.78
1:G:289:GLU:OE1	3:G:401:HOH:O	2.00	0.78
1:C:11:LYS:HG2	3:C:462:HOH:O	1.84	0.78
1:H:14:ARG:NH1	1:H:17:GLN:OE1	2.17	0.77
1:D:231:PRO:O	1:D:234:GLU:HG2	1.83	0.77
1:I:122:ALA:O	3:I:410:HOH:O	2.03	0.77
1:H:110:GLY:HA3	1:I:197:MET:HE1	1.67	0.76
1:D:52:VAL:O	3:D:419:HOH:O	2.02	0.76
1:D:229:LYS:HA	1:D:255:ASN:ND2	2.00	0.76
1:E:58:HIS:NE2	3:E:469:HOH:O	2.18	0.76
1:F:246:GLY:O	3:F:444:HOH:O	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:ARG:NH1	1:I:161:ASP:OD1	2.18	0.76
1:D:268:ALA:HA	1:D:285:LEU:HD12	1.68	0.76
1:D:107:ARG:HH12	1:D:140:ALA:HA	1.50	0.76
1:D:252:MET:HG2	1:D:256:ILE:HG13	1.68	0.75
1:D:230:LEU:HB3	1:D:234:GLU:HG3	1.67	0.75
1:E:151:GLN:OE1	3:E:456:HOH:O	2.05	0.75
1:F:271:ALA:HB1	1:F:277:GLU:HG3	1.67	0.75
1:D:254:ARG:HA	1:D:257:PHE:CZ	2.21	0.75
1:H:280:ASP:HA	1:H:283:TYR:CD1	2.21	0.75
1:A:177:GLY:H	1:A:180:MET:HE2	1.52	0.75
1:F:177:GLY:O	1:F:179:ASP:N	2.18	0.74
1:A:192:ARG:NH2	3:A:406:HOH:O	2.19	0.74
1:D:14:ARG:NH1	1:D:17:GLN:OE1	2.20	0.74
1:D:271:ALA:HA	1:D:275:HIS:HB3	1.69	0.74
1:H:58:HIS:NE2	2:H:301:26T:O09	2.19	0.74
1:D:58:HIS:CE1	2:D:301:26T:H5	2.23	0.74
1:H:233:ARG:HA	1:H:283:TYR:CE2	2.23	0.74
1:D:233:ARG:CD	1:D:283:TYR:HB2	2.19	0.73
1:A:235:ALA:HA	1:A:238:MET:HE3	1.69	0.73
1:D:215:VAL:HG22	1:D:222:ILE:HG21	1.71	0.73
1:D:155:ASN:OD1	3:D:433:HOH:O	2.06	0.73
1:B:197:MET:HE1	1:E:110:GLY:HA3	1.70	0.73
1:D:252:MET:HE2	1:D:256:ILE:HG12	1.71	0.72
1:D:256:ILE:CB	1:D:265:MET:SD	2.77	0.72
1:F:212:GLU:HG2	1:F:245:GLN:HB3	1.71	0.72
1:G:88:THR:O	3:G:427:HOH:O	2.06	0.72
1:I:277:GLU:OE1	3:I:401:HOH:O	2.05	0.72
1:A:229:LYS:NZ	1:A:230:LEU:O	2.21	0.72
1:A:207:VAL:O	1:A:211:PHE:HB2	1.89	0.71
1:D:50:LYS:HA	1:D:248:SER:O	1.89	0.71
1:D:54:LEU:HB2	1:D:266:MET:HE1	1.72	0.71
1:C:14:ARG:NH2	3:C:436:HOH:O	2.23	0.71
1:D:66:THR:HG1	1:D:258:GLN:HE21	1.38	0.71
1:G:87:CYS:SG	3:G:427:HOH:O	2.47	0.71
1:D:252:MET:CE	1:D:256:ILE:HG12	2.20	0.71
1:K:71:ILE:HA	1:K:75:ILE:HG22	1.71	0.71
1:H:171:MET:SD	3:H:435:HOH:O	2.47	0.71
1:A:197:MET:O	3:A:439:HOH:O	2.08	0.71
1:C:285:LEU:HG	1:C:288:SER:HB3	1.71	0.71
1:G:288:SER:HB3	3:G:401:HOH:O	1.91	0.71
1:D:224:ILE:HG22	1:D:250:VAL:HG13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:SER:O	3:E:420:HOH:O	2.08	0.70
1:C:70:ARG:HB3	1:C:73:ILE:HB	1.73	0.70
1:K:206:TYR:OH	1:K:208:GLU:OE1	2.08	0.70
1:D:98:PRO:O	3:D:418:HOH:O	2.07	0.70
1:H:81:HIS:HB2	1:H:266:MET:HG2	1.73	0.70
1:G:207:VAL:HG13	3:G:415:HOH:O	1.91	0.70
1:G:200:GLN:NE2	3:G:432:HOH:O	2.20	0.70
1:D:233:ARG:HD3	1:D:283:TYR:CB	2.22	0.70
1:E:213:ARG:HH22	1:K:9:ASP:HA	1.56	0.70
1:D:44:PHE:HZ	1:D:201:ILE:HD13	1.57	0.70
1:G:286:TYR:CD2	1:G:287:LEU:HA	2.26	0.69
1:K:212:GLU:HG2	1:K:245:GLN:HB2	1.73	0.69
1:B:199:ALA:O	3:B:411:HOH:O	2.09	0.69
1:B:83:ASP:OD2	1:B:274:HIS:NE2	2.25	0.69
1:D:67:GLY:O	3:D:412:HOH:O	2.09	0.69
2:E:301:26T:O10	3:E:469:HOH:O	2.09	0.69
1:E:71:ILE:O	1:E:75:ILE:HG22	1.91	0.69
1:D:100:THR:HG22	1:D:102:ARG:HG2	1.75	0.69
1:G:212:GLU:HB3	1:G:245:GLN:HE21	1.57	0.69
1:G:9:ASP:CG	1:G:10:GLY:H	2.01	0.69
1:K:151:GLN:OE1	3:K:442:HOH:O	2.12	0.68
1:D:232:GLU:OE2	1:D:260:ASP:N	2.26	0.68
1:B:22:ILE:O	3:B:416:HOH:O	2.12	0.68
1:K:228:LYS:HA	1:K:254:ARG:NH2	2.08	0.68
1:D:222:ILE:HG23	1:D:247:ALA:HA	1.74	0.68
1:E:208:GLU:O	3:E:450:HOH:O	2.12	0.68
1:H:81:HIS:CE1	1:H:263:VAL:HG13	2.29	0.67
1:A:117:GLU:OE1	1:A:119:SER:N	2.27	0.67
1:A:266:MET:O	1:A:270:GLN:N	2.27	0.67
1:E:62:GLN:HG2	1:E:114:ILE:HD11	1.77	0.67
1:K:264:ALA:HA	1:K:267:LYS:HG3	1.76	0.66
1:C:266:MET:O	1:C:270:GLN:HG3	1.94	0.66
1:G:58:HIS:CE1	2:G:301:26T:H5	2.30	0.66
1:C:231:PRO:HD2	1:C:234:GLU:HB3	1.75	0.66
1:G:64:PRO:HG2	1:H:188:SER:HB3	1.77	0.66
1:D:252:MET:HE2	1:D:256:ILE:CG1	2.25	0.66
1:K:187:PHE:HB3	1:K:214:ILE:HD12	1.75	0.66
1:A:125:LEU:HD21	1:A:130:ALA:HB2	1.76	0.66
1:B:141:GLN:NE2	3:B:456:HOH:O	2.18	0.66
1:K:228:LYS:HA	1:K:254:ARG:HH21	1.60	0.66
1:G:128:ASP:OD2	3:G:411:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:O	3:A:442:HOH:O	2.12	0.66
1:D:68:LEU:HD22	1:D:71:ILE:CD1	2.26	0.65
1:G:79:PHE:O	1:G:102:ARG:CZ	2.44	0.65
1:I:81:HIS:CD2	1:I:263:VAL:HG13	2.31	0.65
1:B:110:GLY:HA3	1:C:197:MET:HE1	1.79	0.65
1:D:265:MET:HG3	1:D:266:MET:H	1.61	0.65
1:K:244:ASP:OD2	3:K:434:HOH:O	2.14	0.65
1:A:197:MET:HE1	1:D:110:GLY:HA3	1.78	0.65
1:B:289:GLU:OE1	3:B:462:HOH:O	2.13	0.65
1:D:165:LYS:O	1:G:132:ARG:NH2	2.30	0.65
1:B:229:LYS:NZ	1:B:230:LEU:O	2.28	0.65
1:G:58:HIS:HE1	2:G:301:26T:H5	1.62	0.65
1:H:280:ASP:HA	1:H:283:TYR:CE1	2.30	0.64
1:D:95:VAL:HG12	1:G:19:GLN:HE21	1.62	0.64
1:C:120:ASN:OD1	3:C:450:HOH:O	2.14	0.64
1:I:143:TYR:HA	1:I:175:GLY:O	1.98	0.64
1:A:58:HIS:NE2	2:A:301:26T:O09	2.30	0.64
1:B:74:ASN:N	1:B:74:ASN:ND2	2.38	0.64
1:B:78:LEU:HD21	1:B:262:PRO:HB2	1.78	0.64
1:K:241:GLN:O	1:K:245:GLN:HG2	1.97	0.64
1:D:9:ASP:N	3:D:414:HOH:O	2.31	0.64
1:H:117:GLU:O	3:H:429:HOH:O	2.15	0.64
1:A:212:GLU:HG2	1:A:245:GLN:HB3	1.79	0.64
1:K:191:THR:HG21	1:K:214:ILE:HD11	1.79	0.64
1:D:170:THR:OG1	3:D:406:HOH:O	2.15	0.64
1:D:144:ILE:HD12	1:D:190:ALA:HA	1.80	0.64
1:E:49:GLY:HA2	3:E:426:HOH:O	1.97	0.64
1:K:238:MET:SD	3:K:424:HOH:O	2.55	0.64
1:D:233:ARG:HD3	1:D:283:TYR:CG	2.33	0.63
1:H:252:MET:HG2	1:H:256:ILE:HG12	1.78	0.63
1:D:17:GLN:O	1:G:70:ARG:NH1	2.31	0.63
1:C:124:ALA:HA	1:D:157:ILE:HD13	1.80	0.63
1:D:256:ILE:CG1	1:D:265:MET:SD	2.86	0.63
1:K:227:GLY:O	1:K:254:ARG:NH2	2.31	0.63
1:C:70:ARG:NH2	1:H:17:GLN:O	2.32	0.63
1:A:14:ARG:HG3	1:K:70:ARG:HD2	1.80	0.63
1:D:11:LYS:O	1:H:213:ARG:NH2	2.32	0.63
1:D:252:MET:CE	1:D:265:MET:HE1	2.24	0.63
1:K:78:LEU:HB3	1:K:266:MET:HE1	1.79	0.63
1:K:252:MET:HB3	1:K:256:ILE:HD11	1.81	0.63
1:A:78:LEU:CB	1:A:266:MET:HE1	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:229:LYS:HA	1:K:255:ASN:OD1	1.99	0.63
1:D:262:PRO:HA	1:D:265:MET:HG2	1.81	0.63
1:K:211:PHE:HB3	1:K:245:GLN:NE2	2.13	0.63
1:D:174:THR:CG2	1:D:190:ALA:HB1	2.29	0.62
1:I:82:ALA:HB2	1:I:266:MET:HE1	1.81	0.62
1:C:240:TRP:HE3	1:C:241:GLN:HG3	1.63	0.62
1:D:11:LYS:HD3	1:H:185:ARG:HH21	1.64	0.62
1:B:117:GLU:O	3:B:424:HOH:O	2.16	0.62
1:D:81:HIS:O	1:D:81:HIS:ND1	2.32	0.62
1:D:204:THR:HG21	1:D:214:ILE:HD11	1.82	0.62
1:E:71:ILE:HG23	1:E:75:ILE:HG21	1.81	0.62
1:I:213:ARG:NH1	3:I:447:HOH:O	2.32	0.62
1:K:182:ARG:HH11	1:K:182:ARG:HG3	1.65	0.62
1:H:283:TYR:HA	1:H:286:TYR:HB3	1.82	0.62
1:D:29:CYS:O	1:D:37:GLN:NE2	2.31	0.62
1:E:263:VAL:O	1:E:267:LYS:HG2	1.99	0.61
1:B:270:GLN:HG2	1:B:274:HIS:HD2	1.65	0.61
1:A:9:ASP:C	1:A:11:LYS:H	2.06	0.61
1:E:132:ARG:O	1:F:35:GLY:HA3	2.00	0.61
1:F:136:CYS:SG	3:F:475:HOH:O	2.56	0.61
1:K:177:GLY:HA3	1:K:180:MET:HG2	1.81	0.61
1:K:27:LYS:O	1:K:221:PRO:HD3	2.01	0.61
1:D:53:MET:HB3	1:D:251:ASP:HA	1.82	0.60
1:F:183:ASP:OD2	3:F:446:HOH:O	2.16	0.60
1:I:80:GLU:HG3	1:I:81:HIS:CE1	2.36	0.60
1:K:45:ASN:OD1	1:K:47:LYS:HB2	2.01	0.60
1:A:155:ASN:OD1	3:A:432:HOH:O	2.17	0.60
1:E:180:MET:SD	3:E:465:HOH:O	2.57	0.60
1:H:184:GLN:HG3	3:H:440:HOH:O	1.99	0.60
1:C:70:ARG:NE	1:H:13:PHE:O	2.32	0.60
1:F:263:VAL:HG12	1:F:267:LYS:NZ	2.16	0.60
1:I:176:VAL:HG22	1:I:178:LYS:CD	2.28	0.60
1:H:283:TYR:HA	1:H:286:TYR:CB	2.31	0.60
1:E:27:LYS:O	1:E:221:PRO:HD3	2.01	0.60
1:B:33:ASP:OD2	1:I:93:ARG:NH1	2.35	0.60
1:B:20:LYS:HG3	3:B:404:HOH:O	2.02	0.60
1:D:70:ARG:NH1	1:G:13:PHE:O	2.28	0.60
1:D:254:ARG:CA	1:D:257:PHE:CZ	2.85	0.60
1:H:236:LEU:HD12	1:H:283:TYR:CE2	2.36	0.60
1:I:264:ALA:HB2	1:I:289:GLU:HB2	1.84	0.60
1:C:11:LYS:HB2	1:C:13:PHE:HE1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LYS:HD3	1:D:255:ASN:HA	1.84	0.59
1:H:55:ALA:HA	1:H:86:MET:HB3	1.84	0.59
1:C:53:MET:HB3	1:C:251:ASP:HA	1.84	0.59
1:D:34:TRP:NE1	1:G:96:VAL:O	2.26	0.59
1:D:89:ARG:NH1	1:D:129:ASP:OD2	2.34	0.59
1:E:92:LEU:HD22	1:E:106:LEU:HD21	1.84	0.59
1:G:199:ALA:O	3:G:444:HOH:O	2.17	0.59
1:D:95:VAL:HG12	1:G:19:GLN:NE2	2.18	0.59
1:E:252:MET:SD	1:E:255:ASN:HB2	2.42	0.59
1:K:256:ILE:O	1:K:259:SER:OG	2.19	0.59
1:A:144:ILE:HD12	1:A:190:ALA:HA	1.85	0.59
1:B:82:ALA:HB2	1:B:266:MET:HE1	1.85	0.59
1:B:144:ILE:HG22	1:E:115:LEU:HD12	1.85	0.59
1:E:233:ARG:NH1	3:E:403:HOH:O	2.36	0.59
1:I:27:LYS:O	1:I:221:PRO:HD3	2.03	0.59
1:B:278:THR:OG1	1:B:281:ARG:HB2	2.02	0.58
1:H:233:ARG:CZ	1:H:283:TYR:HB2	2.33	0.58
1:I:177:GLY:H	1:I:180:MET:HE3	1.67	0.58
1:K:107:ARG:HH12	1:K:141:GLN:HG2	1.68	0.58
1:A:73:ILE:HG22	1:A:74:ASN:OD1	2.04	0.58
1:I:278:THR:OG1	1:I:281:ARG:HB2	2.03	0.58
1:A:14:ARG:HD2	1:K:74:ASN:HD21	1.68	0.58
1:D:256:ILE:HG12	1:D:265:MET:SD	2.43	0.58
1:E:101:ASN:OD1	3:E:437:HOH:O	2.17	0.58
1:C:240:TRP:CE3	1:C:241:GLN:HG3	2.38	0.58
1:D:235:ALA:O	1:D:238:MET:HB3	2.04	0.58
1:F:42:ARG:HB2	3:F:475:HOH:O	2.03	0.58
1:F:215:VAL:HG11	1:F:246:GLY:HA3	1.86	0.58
1:D:44:PHE:CZ	1:D:201:ILE:HD13	2.38	0.58
1:G:189:LEU:O	1:G:193:ILE:HG12	2.03	0.58
1:I:110:GLY:N	3:I:410:HOH:O	2.14	0.58
1:B:88:THR:HG22	1:B:107:ARG:HB3	1.86	0.58
1:D:235:ALA:HB1	1:D:238:MET:HB2	1.85	0.58
1:A:178:LYS:HA	3:A:401:HOH:O	2.04	0.57
1:E:206:TYR:HB3	1:E:238:MET:HE3	1.86	0.57
1:C:42:ARG:HB3	1:C:103:PRO:HG3	1.85	0.57
1:I:67:GLY:N	1:I:69:GLU:OE2	2.30	0.57
1:E:42:ARG:NH2	3:E:439:HOH:O	2.37	0.57
1:I:53:MET:HG3	1:I:84:VAL:HG13	1.87	0.57
1:C:73:ILE:HG21	1:H:14:ARG:HD3	1.87	0.57
1:C:281:ARG:HA	1:C:284:GLU:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASN:ND2	3:D:429:HOH:O	2.37	0.57
1:G:204:THR:HG22	1:G:205:TYR:H	1.69	0.57
1:K:256:ILE:HG21	1:K:266:MET:HE2	1.86	0.57
1:D:261:HIS:N	1:D:262:PRO:HD3	2.19	0.57
1:C:9:ASP:N	3:C:462:HOH:O	2.37	0.57
1:C:236:LEU:HD12	1:C:265:MET:HE1	1.86	0.57
1:B:226:GLY:HA3	3:B:452:HOH:O	2.05	0.57
1:C:128:ASP:OD1	1:C:132:ARG:NH1	2.26	0.57
1:F:27:LYS:O	1:F:221:PRO:HD3	2.05	0.57
1:D:174:THR:HG21	1:D:190:ALA:CB	2.33	0.56
1:G:278:THR:HG1	1:G:281:ARG:CG	1.95	0.56
1:D:184:GLN:HG3	1:D:210:GLY:O	2.04	0.56
1:K:57:ASP:HB3	1:K:87:CYS:HA	1.86	0.56
1:B:252:MET:HG2	1:B:256:ILE:HG13	1.85	0.56
1:C:88:THR:HG22	1:C:107:ARG:HB3	1.88	0.56
1:C:241:GLN:O	1:C:245:GLN:HG3	2.05	0.56
1:B:239:CYS:SG	1:B:252:MET:HE1	2.46	0.56
1:D:19:GLN:HB3	1:H:27:LYS:HD2	1.88	0.56
1:D:26:LEU:O	1:H:21:ASN:ND2	2.34	0.56
1:A:277:GLU:OE2	1:A:278:THR:N	2.39	0.56
1:A:184:GLN:HE21	1:A:214:ILE:HG13	1.71	0.56
1:F:266:MET:O	1:F:270:GLN:HG2	2.05	0.56
1:G:88:THR:HG22	1:G:107:ARG:HB3	1.88	0.56
1:K:232:GLU:O	1:K:236:LEU:HD12	2.05	0.56
1:F:229:LYS:NZ	1:F:230:LEU:O	2.37	0.56
1:F:277:GLU:OE1	1:F:281:ARG:HB3	2.06	0.56
1:G:144:ILE:HD13	1:G:190:ALA:HA	1.88	0.56
1:A:233:ARG:NH2	1:A:283:TYR:HB3	2.21	0.55
1:K:88:THR:HG22	1:K:107:ARG:HB3	1.87	0.55
1:B:124:ALA:HA	1:C:157:ILE:HD13	1.87	0.55
1:D:228:LYS:HA	1:D:254:ARG:HE	1.72	0.55
1:D:270:GLN:HB2	1:D:274:HIS:NE2	2.20	0.55
1:C:236:LEU:CD1	1:C:265:MET:HE1	2.36	0.55
1:D:234:GLU:O	1:D:236:LEU:N	2.29	0.55
1:C:14:ARG:HD3	1:C:17:GLN:NE2	2.21	0.55
1:G:107:ARG:NH2	1:G:141:GLN:OE1	2.35	0.55
1:H:285:LEU:HA	1:H:288:SER:HB3	1.88	0.55
1:H:226:GLY:HA3	3:H:438:HOH:O	2.07	0.55
1:A:64:PRO:O	1:K:11:LYS:HD3	2.07	0.55
1:K:142:VAL:O	1:K:175:GLY:N	2.30	0.55
1:A:27:LYS:O	1:A:221:PRO:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ILE:CG2	1:A:266:MET:HE2	2.36	0.55
1:D:200:GLN:HA	1:D:220:VAL:HG11	1.88	0.55
1:E:11:LYS:HD3	1:E:13:PHE:CE1	2.42	0.55
1:K:266:MET:O	1:K:270:GLN:HG2	2.06	0.55
1:D:261:HIS:ND1	1:D:287:LEU:HB3	2.22	0.54
1:D:254:ARG:CA	1:D:257:PHE:CE1	2.85	0.54
1:G:256:ILE:C	1:G:258:GLN:H	2.14	0.54
1:E:229:LYS:NZ	1:E:230:LEU:O	2.34	0.54
1:H:80:GLU:HG2	1:H:81:HIS:HD2	1.72	0.54
1:D:13:PHE:HB2	1:H:213:ARG:HG2	1.89	0.54
1:F:215:VAL:HG13	3:F:444:HOH:O	2.06	0.54
1:K:261:HIS:ND1	1:K:287:LEU:HD21	2.22	0.54
1:A:19:GLN:HG2	1:G:27:LYS:HZ3	1.73	0.54
1:C:72:ASP:OD2	1:H:19:GLN:HG3	2.06	0.54
1:D:252:MET:CE	1:D:256:ILE:CG1	2.86	0.54
1:D:256:ILE:CD1	1:D:265:MET:CE	2.84	0.54
1:G:141:GLN:HG2	1:G:143:TYR:CZ	2.42	0.54
1:A:149:GLU:OE2	1:D:113:SER:HB2	2.07	0.54
1:I:263:VAL:O	1:I:267:LYS:HG3	2.08	0.54
1:E:184:GLN:HG3	1:E:210:GLY:O	2.08	0.54
1:H:206:TYR:HB3	1:H:238:MET:HE3	1.88	0.54
1:A:189:LEU:O	1:A:193:ILE:HD12	2.08	0.54
1:K:260:ASP:O	1:K:261:HIS:HD2	1.91	0.54
1:D:256:ILE:CG1	1:D:265:MET:CE	2.79	0.54
1:I:206:TYR:HE1	1:I:245:GLN:OE1	1.91	0.54
1:D:50:LYS:CA	1:D:248:SER:O	2.57	0.53
1:G:258:GLN:NE2	3:G:437:HOH:O	2.40	0.53
1:H:27:LYS:O	1:H:221:PRO:HD3	2.08	0.53
1:C:145:GLY:HA3	1:C:180:MET:HE3	1.90	0.53
1:E:180:MET:O	3:E:401:HOH:O	2.19	0.53
1:F:69:GLU:OE2	3:F:429:HOH:O	2.17	0.53
1:G:254:ARG:O	1:G:258:GLN:HB3	2.08	0.53
1:H:54:LEU:N	3:H:436:HOH:O	2.42	0.53
1:A:19:GLN:HB3	1:K:70:ARG:HH12	1.74	0.53
1:I:93:ARG:NH2	1:I:129:ASP:OD1	2.42	0.53
1:D:34:TRP:CE3	1:G:92:LEU:HD21	2.44	0.53
1:D:117:GLU:CD	1:D:118:LEU:H	2.17	0.53
1:D:270:GLN:HB2	1:D:274:HIS:HE2	1.73	0.53
1:E:252:MET:SD	1:E:256:ILE:HG13	2.49	0.53
1:G:95:VAL:O	3:G:414:HOH:O	2.18	0.53
1:G:267:LYS:HA	1:G:270:GLN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:ARG:HA	1:H:283:TYR:CZ	2.43	0.53
1:H:16:ASP:OD1	1:H:17:GLN:HG3	2.09	0.53
1:I:176:VAL:CG2	1:I:186:TYR:CE2	2.92	0.53
1:A:69:GLU:HG2	1:K:11:LYS:HG2	1.90	0.53
1:D:200:GLN:NE2	3:D:427:HOH:O	2.38	0.53
1:E:101:ASN:HA	3:E:437:HOH:O	2.08	0.53
1:H:117:GLU:OE1	1:H:119:SER:N	2.43	0.53
1:A:104:VAL:HG22	3:A:431:HOH:O	2.09	0.52
1:A:132:ARG:O	1:K:35:GLY:HA3	2.08	0.52
1:G:206:TYR:HB3	1:G:238:MET:HE2	1.92	0.52
1:I:177:GLY:C	1:I:178:LYS:HG2	2.35	0.52
1:B:253:GLY:H	2:B:301:26T:H7	1.55	0.52
1:I:44:PHE:HA	1:I:51:THR:OG1	2.09	0.52
1:K:82:ALA:O	1:K:102:ARG:HD3	2.09	0.52
1:C:224:ILE:HG22	1:C:225:ALA:O	2.09	0.52
1:K:92:LEU:HD22	1:K:106:LEU:HD21	1.91	0.52
1:K:253:GLY:N	2:K:301:26T:O08	2.29	0.52
1:E:182:ARG:HB2	1:E:187:PHE:CZ	2.44	0.52
1:I:287:LEU:O	1:I:289:GLU:N	2.42	0.52
1:A:184:GLN:NE2	1:A:213:ARG:HB2	2.24	0.52
1:A:211:PHE:HB3	1:A:245:GLN:OE1	2.10	0.52
1:H:60:TYR:OH	1:H:121:GLU:OE2	2.23	0.52
1:I:229:LYS:NZ	1:I:230:LEU:O	2.24	0.52
1:A:270:GLN:O	1:A:274:HIS:HB3	2.09	0.52
1:H:144:ILE:O	1:H:186:TYR:OH	2.15	0.52
1:K:107:ARG:NH1	1:K:141:GLN:HG2	2.25	0.52
1:A:88:THR:HG22	1:A:107:ARG:HB3	1.92	0.52
1:G:202:ILE:HB	1:G:222:ILE:HG12	1.92	0.52
1:D:229:LYS:NZ	1:D:232:GLU:HA	2.25	0.51
1:A:157:ILE:HD13	1:D:124:ALA:HA	1.92	0.51
1:B:184:GLN:OE1	1:B:213:ARG:HD3	2.10	0.51
1:G:229:LYS:HG3	1:G:258:GLN:OE1	2.10	0.51
1:H:88:THR:HG22	1:H:107:ARG:HB3	1.92	0.51
1:C:127:MET:HE3	1:C:130:ALA:HB3	1.91	0.51
1:D:68:LEU:HD22	1:D:71:ILE:HD11	1.92	0.51
1:H:93:ARG:NH2	1:H:129:ASP:OD1	2.43	0.51
1:H:236:LEU:HB2	1:H:283:TYR:CZ	2.45	0.51
1:K:206:TYR:HE1	1:K:245:GLN:HE21	1.59	0.51
1:E:53:MET:HB3	1:E:251:ASP:HA	1.93	0.51
1:G:286:TYR:HD2	1:G:287:LEU:HA	1.74	0.51
1:H:184:GLN:OE1	1:H:210:GLY:HA3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:88:THR:HG22	1:I:107:ARG:HB3	1.91	0.51
1:K:53:MET:HB3	1:K:251:ASP:HA	1.91	0.51
1:D:243:ILE:HG13	1:D:273:VAL:HG12	1.92	0.51
1:I:287:LEU:O	1:I:289:GLU:HG2	2.11	0.51
1:A:55:ALA:HB2	1:A:251:ASP:OD1	2.09	0.51
1:A:69:GLU:CD	1:A:69:GLU:H	2.17	0.51
1:A:252:MET:HG2	1:A:256:ILE:HG13	1.91	0.51
1:D:204:THR:HG21	1:D:222:ILE:HD11	1.92	0.51
1:F:50:LYS:HD3	1:F:273:VAL:O	2.11	0.51
1:G:27:LYS:O	1:G:221:PRO:HD3	2.10	0.51
1:B:92:LEU:HD22	1:B:106:LEU:HD21	1.91	0.51
1:I:144:ILE:HG13	1:I:190:ALA:HA	1.92	0.51
1:A:19:GLN:O	3:A:410:HOH:O	2.18	0.51
1:A:192:ARG:HG3	3:D:402:HOH:O	2.11	0.51
1:A:284:GLU:HG2	1:A:284:GLU:O	2.10	0.51
1:C:73:ILE:HG22	1:C:74:ASN:N	2.25	0.50
1:H:124:ALA:HA	1:I:157:ILE:HD13	1.92	0.50
1:I:179:ASP:OD1	1:I:179:ASP:O	2.29	0.50
1:A:102:ARG:NH2	3:A:422:HOH:O	2.43	0.50
1:B:17:GLN:OE1	3:B:453:HOH:O	2.18	0.50
1:F:55:ALA:HA	1:F:86:MET:CB	2.41	0.50
1:F:55:ALA:HA	1:F:86:MET:HB3	1.93	0.50
1:G:252:MET:HG2	1:G:256:ILE:HG13	1.92	0.50
1:H:283:TYR:C	1:H:286:TYR:H	2.19	0.50
1:A:182:ARG:HB2	1:A:187:PHE:CZ	2.46	0.50
1:A:267:LYS:HD2	1:A:289:GLU:OE1	2.11	0.50
1:B:64:PRO:O	1:I:11:LYS:HE2	2.10	0.50
1:C:231:PRO:HD2	1:C:234:GLU:CB	2.42	0.50
1:D:67:GLY:H	1:D:69:GLU:CD	2.20	0.50
1:H:233:ARG:HD3	1:H:283:TYR:CD1	2.46	0.50
1:F:76:ALA:HA	1:F:79:PHE:CE2	2.47	0.50
1:K:211:PHE:HB3	1:K:245:GLN:HE21	1.75	0.50
1:K:260:ASP:O	1:K:261:HIS:CD2	2.64	0.50
1:C:166:VAL:O	1:H:132:ARG:HA	2.11	0.50
1:C:254:ARG:O	1:C:258:GLN:HB2	2.11	0.50
1:D:254:ARG:O	1:D:258:GLN:HB2	2.11	0.50
1:F:264:ALA:HB2	1:F:289:GLU:HB2	1.93	0.50
1:F:264:ALA:CB	1:F:289:GLU:HB2	2.40	0.50
1:A:240:TRP:NE1	1:A:278:THR:HA	2.27	0.50
1:E:254:ARG:HG3	3:E:469:HOH:O	2.11	0.50
1:H:58:HIS:NE2	2:H:301:26T:H5	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLY:HA3	1:I:132:ARG:O	2.10	0.50
1:B:58:HIS:NE2	2:B:301:26T:H5	2.26	0.50
1:E:61:PHE:O	1:E:114:ILE:HG12	2.12	0.50
1:G:57:ASP:HB3	1:G:87:CYS:HA	1.93	0.50
1:A:287:LEU:HD12	1:A:288:SER:N	2.26	0.50
1:C:134:ASN:O	3:C:443:HOH:O	2.20	0.50
1:I:142:VAL:O	1:I:175:GLY:N	2.44	0.50
1:B:216:ALA:HB2	3:B:468:HOH:O	2.11	0.49
1:D:250:VAL:HG12	1:D:252:MET:H	1.77	0.49
1:I:121:GLU:HB3	3:I:410:HOH:O	2.11	0.49
1:A:142:VAL:HA	1:A:152:SER:HB2	1.94	0.49
1:A:233:ARG:HA	1:A:283:TYR:CE1	2.47	0.49
1:F:215:VAL:HA	1:F:222:ILE:HD12	1.95	0.49
1:I:284:GLU:O	1:I:284:GLU:HG2	2.12	0.49
1:K:55:ALA:HB2	1:K:251:ASP:OD1	2.12	0.49
1:E:212:GLU:H	1:E:212:GLU:CD	2.20	0.49
1:C:27:LYS:O	1:C:221:PRO:HD3	2.11	0.49
1:C:213:ARG:NH2	3:C:458:HOH:O	2.45	0.49
1:G:53:MET:HB3	1:G:251:ASP:HA	1.94	0.49
1:G:62:GLN:NE2	3:G:435:HOH:O	2.46	0.49
1:A:243:ILE:HD11	1:A:273:VAL:HG13	1.93	0.49
1:D:132:ARG:HA	1:G:166:VAL:O	2.12	0.49
1:G:72:ASP:OD2	1:G:73:ILE:HG13	2.13	0.49
1:I:176:VAL:HG13	1:I:178:LYS:HE3	1.95	0.49
1:K:42:ARG:HB3	1:K:103:PRO:HG3	1.94	0.49
1:K:254:ARG:HG3	1:K:257:PHE:CZ	2.47	0.49
1:A:17:GLN:OE1	1:K:73:ILE:HD13	2.12	0.49
1:C:224:ILE:HD11	1:C:242:ALA:HB3	1.95	0.49
1:C:241:GLN:HA	1:C:244:ASP:HB3	1.94	0.49
1:H:280:ASP:HA	1:H:283:TYR:HD1	1.75	0.49
1:I:215:VAL:HG11	1:I:246:GLY:HA3	1.94	0.49
1:K:211:PHE:CZ	1:K:224:ILE:HD11	2.47	0.49
1:A:15:THR:HA	3:A:427:HOH:O	2.11	0.49
1:H:200:GLN:OE1	3:H:413:HOH:O	2.20	0.49
1:K:182:ARG:HG3	1:K:182:ARG:NH1	2.25	0.49
1:A:93:ARG:NH2	1:A:129:ASP:OD1	2.45	0.49
1:D:240:TRP:CD1	1:D:277:GLU:O	2.66	0.49
1:D:252:MET:CE	1:D:265:MET:CE	2.89	0.49
1:G:52:VAL:HA	1:G:250:VAL:HG22	1.94	0.49
1:G:184:GLN:C	1:G:184:GLN:OE1	2.55	0.49
1:C:239:CYS:SG	1:C:252:MET:HE1	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:GLU:OE2	1:D:281:ARG:HB3	2.12	0.49
1:A:12:ASP:OD2	3:A:424:HOH:O	2.20	0.48
1:F:53:MET:HG3	1:F:84:VAL:HG13	1.95	0.48
1:G:82:ALA:N	1:G:102:ARG:HH22	2.11	0.48
1:I:176:VAL:HG23	1:I:186:TYR:CZ	2.47	0.48
1:K:175:GLY:O	3:K:428:HOH:O	2.20	0.48
1:B:93:ARG:NH2	1:B:129:ASP:OD1	2.46	0.48
1:H:73:ILE:HG22	1:H:74:ASN:OD1	2.13	0.48
1:I:93:ARG:O	3:I:409:HOH:O	2.20	0.48
1:K:239:CYS:SG	1:K:252:MET:HE1	2.52	0.48
1:D:222:ILE:O	1:D:248:SER:N	2.36	0.48
1:D:252:MET:HE2	1:D:265:MET:CE	2.31	0.48
1:D:78:LEU:HD11	1:D:262:PRO:HB2	1.96	0.48
1:F:227:GLY:N	2:F:301:26T:O10	2.45	0.48
1:G:254:ARG:HA	1:G:257:PHE:CZ	2.48	0.48
1:B:106:LEU:HB3	1:B:125:LEU:HD21	1.96	0.48
1:B:132:ARG:O	1:I:35:GLY:HA3	2.13	0.48
1:C:132:ARG:NH2	1:H:165:LYS:O	2.47	0.48
1:D:93:ARG:HE	1:D:133:LEU:HD11	1.78	0.48
1:D:254:ARG:HA	1:D:257:PHE:CD1	2.49	0.48
1:E:211:PHE:HB3	1:E:245:GLN:OE1	2.13	0.48
1:B:103:PRO:HB3	1:B:136:CYS:SG	2.54	0.48
1:I:50:LYS:NZ	3:I:451:HOH:O	2.46	0.48
1:I:176:VAL:HG23	1:I:186:TYR:CE2	2.48	0.48
1:A:124:ALA:HA	1:E:157:ILE:HD13	1.94	0.48
1:A:165:LYS:NZ	1:D:128:ASP:OD2	2.39	0.48
1:D:261:HIS:CE1	1:D:287:LEU:HB3	2.48	0.48
1:H:238:MET:N	3:H:441:HOH:O	2.04	0.48
1:I:215:VAL:HA	1:I:222:ILE:HD12	1.95	0.48
1:I:58:HIS:NE2	2:I:301:26T:H5	2.29	0.48
1:I:199:ALA:O	3:I:437:HOH:O	2.20	0.48
1:A:184:GLN:HE22	1:A:213:ARG:HB2	1.78	0.48
1:B:98:PRO:HG3	1:I:34:TRP:CD1	2.49	0.48
1:D:215:VAL:HG22	1:D:222:ILE:HD13	1.96	0.48
1:H:55:ALA:HB2	1:H:251:ASP:OD1	2.14	0.48
1:K:54:LEU:HD21	1:K:75:ILE:HD11	1.96	0.47
1:B:144:ILE:HG13	1:B:190:ALA:HA	1.96	0.47
1:A:48:THR:O	1:A:50:LYS:HD2	2.14	0.47
1:B:241:GLN:O	1:B:245:GLN:HG3	2.14	0.47
1:D:121:GLU:OE2	1:D:143:TYR:OH	2.32	0.47
1:F:157:ILE:HD13	1:I:124:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:LYS:HD2	1:G:273:VAL:O	2.14	0.47
1:K:204:THR:HG21	1:K:214:ILE:HD13	1.96	0.47
1:E:143:TYR:HB3	1:E:146:SER:HB2	1.95	0.47
1:G:89:ARG:NH1	1:G:129:ASP:OD2	2.35	0.47
1:I:287:LEU:C	1:I:289:GLU:H	2.22	0.47
1:K:228:LYS:HD2	1:K:229:LYS:H	1.79	0.47
1:A:182:ARG:O	3:A:428:HOH:O	2.20	0.47
1:A:213:ARG:HD2	1:G:13:PHE:CE1	2.50	0.47
1:C:27:LYS:NZ	3:C:435:HOH:O	2.35	0.47
1:C:33:ASP:OD1	1:H:93:ARG:NH1	2.47	0.47
1:D:13:PHE:HZ	1:H:185:ARG:NH2	2.13	0.47
1:F:218:CYS:HA	1:F:219:PRO:HD3	1.77	0.47
1:G:92:LEU:N	3:G:427:HOH:O	2.47	0.47
1:A:269:VAL:O	1:A:273:VAL:HG23	2.14	0.47
1:C:143:TYR:HB3	1:C:146:SER:HB2	1.96	0.47
1:C:254:ARG:HG3	1:C:257:PHE:CZ	2.50	0.47
1:G:231:PRO:HA	3:G:437:HOH:O	2.13	0.47
1:K:184:GLN:HG3	1:K:213:ARG:HG3	1.96	0.47
1:A:259:SER:N	3:A:442:HOH:O	2.47	0.47
1:C:102:ARG:NH1	3:C:424:HOH:O	2.48	0.47
1:C:232:GLU:O	1:C:236:LEU:HD13	2.15	0.47
1:D:256:ILE:HD13	1:D:265:MET:CE	2.45	0.47
1:E:11:LYS:HD3	1:E:13:PHE:HE1	1.80	0.47
1:H:36:MET:HE3	1:H:167:GLY:HA2	1.97	0.47
1:H:42:ARG:HB3	1:H:103:PRO:HG3	1.96	0.47
1:H:80:GLU:HG2	1:H:81:HIS:CD2	2.50	0.47
1:H:232:GLU:O	1:H:283:TYR:HE2	1.97	0.47
1:D:261:HIS:N	1:D:262:PRO:CD	2.78	0.47
1:K:266:MET:O	1:K:270:GLN:N	2.31	0.47
1:D:98:PRO:HG3	1:G:34:TRP:CD1	2.50	0.47
1:D:229:LYS:HZ1	1:D:232:GLU:HA	1.79	0.47
1:E:33:ASP:OD1	1:F:93:ARG:NH1	2.48	0.47
1:E:132:ARG:NH2	1:F:165:LYS:O	2.48	0.47
1:A:80:GLU:HA	1:A:102:ARG:CZ	2.45	0.46
1:B:218:CYS:HA	1:B:219:PRO:HD3	1.76	0.46
1:D:11:LYS:HD3	1:H:185:ARG:NH2	2.30	0.46
1:H:114:ILE:HA	1:H:118:LEU:HD21	1.97	0.46
1:K:71:ILE:HG23	1:K:75:ILE:CG2	2.45	0.46
1:B:57:ASP:HB3	1:B:87:CYS:HA	1.97	0.46
1:C:265:MET:O	1:C:269:VAL:HG23	2.15	0.46
1:D:256:ILE:HA	1:D:265:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:280:ASP:HB2	1:G:283:TYR:CD2	2.50	0.46
1:K:176:VAL:HG22	1:K:177:GLY:O	2.15	0.46
1:A:69:GLU:CG	1:K:11:LYS:HG2	2.45	0.46
1:C:132:ARG:HA	1:H:166:VAL:O	2.14	0.46
1:D:192:ARG:HD3	1:D:217:GLY:O	2.15	0.46
1:G:157:ILE:HD13	1:K:124:ALA:HA	1.96	0.46
1:I:117:GLU:O	3:I:449:HOH:O	2.21	0.46
1:B:254:ARG:O	1:B:258:GLN:HB2	2.16	0.46
1:H:239:CYS:SG	1:H:252:MET:HE1	2.55	0.46
1:C:278:THR:HB	1:C:281:ARG:HG2	1.97	0.46
1:H:211:PHE:HD2	1:H:245:GLN:HG2	1.79	0.46
1:B:132:ARG:HA	1:I:166:VAL:O	2.15	0.46
1:G:107:ARG:HD2	1:G:107:ARG:HA	1.74	0.46
1:C:82:ALA:HB2	1:C:266:MET:HE1	1.97	0.46
1:D:34:TRP:CD2	1:G:92:LEU:HD21	2.51	0.46
1:F:46:PRO:O	3:F:462:HOH:O	2.20	0.46
1:G:86:MET:HE1	1:G:107:ARG:HH11	1.81	0.46
1:G:107:ARG:NH2	1:G:141:GLN:HB2	2.31	0.46
1:H:43:ILE:HG23	1:H:84:VAL:HG21	1.98	0.46
1:I:33:ASP:OD2	3:I:415:HOH:O	2.21	0.46
1:E:34:TRP:CD1	1:F:98:PRO:HG3	2.51	0.46
1:E:35:GLY:HA3	1:F:132:ARG:O	2.15	0.46
1:G:19:GLN:OE1	1:G:20:LYS:N	2.49	0.46
1:G:76:ALA:HA	1:G:79:PHE:CE2	2.50	0.46
1:G:280:ASP:CB	1:G:283:TYR:HD2	2.29	0.46
1:H:224:ILE:HD12	1:H:238:MET:HE2	1.97	0.46
1:K:50:LYS:HD3	1:K:243:ILE:HD12	1.97	0.46
1:K:177:GLY:HA2	1:K:178:LYS:HB2	1.97	0.46
1:C:278:THR:HB	1:C:281:ARG:CG	2.46	0.46
1:D:61:PHE:CE1	2:D:301:26T:H3	2.51	0.46
1:E:241:GLN:O	1:E:245:GLN:HG3	2.15	0.46
1:F:83:ASP:OD2	1:F:274:HIS:NE2	2.44	0.46
1:C:243:ILE:CD1	1:C:273:VAL:HA	2.45	0.46
1:D:229:LYS:CD	1:D:255:ASN:HA	2.46	0.46
1:D:277:GLU:OE1	1:D:277:GLU:HA	2.15	0.46
1:F:233:ARG:HG3	1:F:233:ARG:O	2.14	0.46
1:G:277:GLU:OE1	1:G:277:GLU:HA	2.15	0.46
1:A:241:GLN:O	1:A:245:GLN:HG3	2.15	0.45
1:D:53:MET:HG3	1:D:84:VAL:HG13	1.98	0.45
2:H:301:26T:O13	3:H:425:HOH:O	2.20	0.45
1:A:277:GLU:OE2	1:A:281:ARG:HD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LEU:CB	1:D:234:GLU:HG3	2.42	0.45
1:G:276:ASN:CA	3:G:419:HOH:O	2.53	0.45
1:E:62:GLN:OE1	1:E:65:THR:HG21	2.16	0.45
1:H:283:TYR:CA	1:H:286:TYR:HB3	2.45	0.45
1:I:58:HIS:NE2	2:I:301:26T:O09	2.34	0.45
1:B:229:LYS:NZ	3:B:463:HOH:O	2.49	0.45
1:E:50:LYS:HA	1:E:248:SER:O	2.16	0.45
1:E:118:LEU:HD23	1:E:177:GLY:HA2	1.98	0.45
1:I:36:MET:HE3	1:I:167:GLY:HA2	1.97	0.45
1:I:142:VAL:HG13	1:I:174:THR:HA	1.99	0.45
1:D:132:ARG:O	1:G:35:GLY:HA3	2.16	0.45
1:D:171:MET:HB2	1:D:201:ILE:HG23	1.97	0.45
1:G:39:ARG:NH1	1:G:167:GLY:O	2.49	0.45
1:I:122:ALA:N	3:I:410:HOH:O	2.49	0.45
1:I:283:TYR:O	1:I:286:TYR:HB3	2.15	0.45
1:E:265:MET:O	1:E:269:VAL:HG23	2.16	0.45
1:G:45:ASN:OD1	1:G:47:LYS:HD2	2.17	0.45
1:I:265:MET:O	1:I:269:VAL:HG23	2.16	0.45
1:B:64:PRO:HG2	1:C:188:SER:HB3	1.98	0.45
1:E:233:ARG:NH2	3:E:402:HOH:O	2.50	0.45
1:C:73:ILE:HG21	1:H:14:ARG:NH1	2.32	0.45
1:E:215:VAL:HA	1:E:222:ILE:HD12	1.99	0.45
1:I:80:GLU:HA	1:I:102:ARG:HE	1.82	0.45
1:A:240:TRP:CD1	1:A:278:THR:HA	2.52	0.45
1:B:27:LYS:O	1:B:221:PRO:HD3	2.17	0.45
1:G:92:LEU:CD2	1:G:133:LEU:HD22	2.47	0.45
1:D:45:ASN:OD1	1:D:47:LYS:HB2	2.17	0.45
1:D:55:ALA:HB2	1:D:251:ASP:OD1	2.17	0.45
1:E:26:LEU:HD13	3:E:426:HOH:O	2.16	0.45
1:E:144:ILE:HD13	1:E:190:ALA:HA	1.99	0.45
1:G:40:LEU:O	1:G:43:ILE:HG13	2.17	0.45
1:G:185:ARG:HH12	1:G:189:LEU:HD11	1.80	0.45
1:C:199:ALA:O	3:C:430:HOH:O	2.21	0.44
1:D:235:ALA:HB1	1:D:238:MET:CB	2.46	0.44
1:G:275:HIS:CD2	1:G:275:HIS:O	2.70	0.44
1:H:88:THR:HB	3:H:417:HOH:O	2.17	0.44
1:D:55:ALA:HA	1:D:86:MET:HB3	2.00	0.44
1:D:270:GLN:HG3	1:D:271:ALA:N	2.32	0.44
1:F:241:GLN:O	1:F:245:GLN:HG3	2.18	0.44
1:F:271:ALA:HB1	1:F:277:GLU:CG	2.42	0.44
1:H:215:VAL:HA	1:H:222:ILE:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:262:PRO:O	1:I:266:MET:HG3	2.17	0.44
1:K:268:ALA:HB2	1:K:286:TYR:HB2	1.99	0.44
1:B:143:TYR:HB3	1:B:146:SER:HB2	1.98	0.44
1:C:230:LEU:HB3	1:C:231:PRO:HD2	1.99	0.44
1:D:212:GLU:CD	1:D:212:GLU:H	2.25	0.44
1:E:166:VAL:O	1:F:132:ARG:HA	2.17	0.44
1:F:88:THR:HG22	1:F:107:ARG:HB3	2.00	0.44
1:F:228:LYS:NZ	1:F:229:LYS:O	2.45	0.44
1:I:42:ARG:NH2	3:I:480:HOH:O	2.31	0.44
1:I:61:PHE:CE2	1:I:118:LEU:HD11	2.52	0.44
1:I:203:ALA:HA	1:I:223:VAL:O	2.17	0.44
1:C:252:MET:HE3	1:C:252:MET:HB2	1.90	0.44
1:D:252:MET:HE3	1:D:256:ILE:HG12	1.95	0.44
1:F:58:HIS:HB2	1:F:68:LEU:HD12	1.99	0.44
1:G:111:ALA:HA	1:H:153:ILE:HG21	2.00	0.44
1:G:165:LYS:HG2	1:K:128:ASP:OD2	2.18	0.44
1:G:184:GLN:HG3	1:G:210:GLY:HA3	1.99	0.44
1:C:15:THR:HG21	1:I:212:GLU:HG2	1.99	0.44
1:D:274:HIS:CE1	1:D:275:HIS:HB2	2.53	0.44
1:A:115:LEU:HD12	1:E:144:ILE:HG22	1.99	0.44
1:C:60:TYR:HA	1:D:196:GLU:HG2	1.98	0.44
1:G:178:LYS:HD3	1:G:178:LYS:HA	1.82	0.44
1:H:81:HIS:CE1	1:H:263:VAL:CG1	2.99	0.44
1:I:276:ASN:HA	3:I:461:HOH:O	2.17	0.44
1:K:215:VAL:HA	1:K:222:ILE:HD12	1.99	0.44
1:A:112:ASN:HB3	1:A:120:ASN:O	2.18	0.44
1:C:61:PHE:HB2	1:C:113:SER:HA	2.00	0.44
1:E:206:TYR:HE2	1:E:208:GLU:HG2	1.82	0.44
1:G:82:ALA:O	1:G:102:ARG:CZ	2.66	0.44
1:A:60:TYR:HB2	1:E:197:MET:HE3	1.99	0.44
1:A:230:LEU:H	1:A:255:ASN:ND2	2.15	0.44
1:D:22:ILE:HA	1:D:23:PRO:HD3	1.79	0.44
1:H:115:LEU:HD12	1:I:144:ILE:HG22	1.99	0.44
1:A:218:CYS:HA	1:A:219:PRO:HD3	1.72	0.44
1:A:266:MET:O	1:A:270:GLN:HB2	2.17	0.44
1:B:9:ASP:N	3:B:405:HOH:O	2.51	0.44
1:I:81:HIS:ND1	1:I:81:HIS:N	2.65	0.44
1:B:55:ALA:HB2	1:B:251:ASP:OD1	2.17	0.43
1:B:111:ALA:O	1:C:150:HIS:ND1	2.38	0.43
1:G:184:GLN:OE1	1:G:185:ARG:N	2.51	0.43
1:B:264:ALA:HB2	1:B:289:GLU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:ARG:HG3	1:E:103:PRO:HD2	1.99	0.43
1:H:79:PHE:HB3	1:H:100:THR:HG21	2.00	0.43
1:I:55:ALA:HB3	2:I:301:26T:H6	1.99	0.43
1:K:45:ASN:HA	1:K:46:PRO:HD3	1.78	0.43
1:K:112:ASN:HB2	1:K:118:LEU:HA	1.99	0.43
1:G:36:MET:HE3	1:G:167:GLY:HA2	2.00	0.43
1:H:81:HIS:ND1	1:H:263:VAL:HG13	2.32	0.43
1:H:278:THR:OG1	1:H:281:ARG:NE	2.51	0.43
1:I:265:MET:HA	1:I:286:TYR:HD1	1.83	0.43
1:A:166:VAL:O	1:K:132:ARG:HA	2.17	0.43
1:E:253:GLY:HA3	3:E:469:HOH:O	2.18	0.43
1:E:264:ALA:HB2	1:E:289:GLU:HB2	1.99	0.43
1:G:193:ILE:HD13	1:K:59:GLY:O	2.18	0.43
1:G:266:MET:O	1:G:270:GLN:N	2.37	0.43
1:H:229:LYS:HA	1:H:255:ASN:OD1	2.19	0.43
1:C:269:VAL:O	1:C:273:VAL:HG23	2.18	0.43
1:D:218:CYS:HA	1:D:219:PRO:HD3	1.69	0.43
1:H:192:ARG:NE	1:H:217:GLY:O	2.51	0.43
1:H:281:ARG:HA	1:H:284:GLU:CB	2.48	0.43
1:C:89:ARG:NH2	1:D:161:ASP:OD1	2.47	0.43
1:D:166:VAL:O	1:G:132:ARG:HA	2.18	0.43
1:H:78:LEU:HD21	1:H:262:PRO:HB2	2.00	0.43
1:I:14:ARG:HG3	1:I:16:ASP:OD1	2.18	0.43
1:A:16:ASP:OD1	1:A:17:GLN:HG3	2.18	0.43
1:D:176:VAL:HG23	1:D:205:TYR:CE2	2.53	0.43
1:D:265:MET:HE2	1:D:266:MET:CA	2.48	0.43
1:F:180:MET:HE2	1:F:180:MET:HB3	1.85	0.43
1:F:211:PHE:HB3	1:F:245:GLN:OE1	2.18	0.43
1:F:262:PRO:O	1:F:266:MET:HG3	2.18	0.43
1:G:204:THR:HG22	1:G:205:TYR:N	2.34	0.43
1:H:45:ASN:OD1	1:H:46:PRO:HD2	2.19	0.43
1:K:93:ARG:NH2	1:K:129:ASP:OD1	2.52	0.43
1:C:11:LYS:HB2	1:C:13:PHE:CE1	2.50	0.43
1:H:184:GLN:HG3	1:H:184:GLN:H	1.55	0.43
1:H:273:VAL:HG21	3:H:443:HOH:O	2.18	0.43
1:K:50:LYS:HD2	1:K:273:VAL:O	2.19	0.43
1:B:33:ASP:HB2	1:F:33:ASP:HB2	2.01	0.43
1:B:157:ILE:HD13	1:E:124:ALA:HA	2.01	0.43
1:C:206:TYR:HB3	1:C:238:MET:HE3	2.01	0.43
1:C:224:ILE:O	1:C:251:ASP:N	2.32	0.43
1:E:43:ILE:HG23	1:E:84:VAL:HG11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:206:TYR:CE1	1:I:245:GLN:OE1	2.71	0.43
1:K:70:ARG:CD	1:K:73:ILE:HD12	2.49	0.43
1:C:173:VAL:HG22	1:C:203:ALA:HB3	2.01	0.43
1:F:50:LYS:NZ	3:F:427:HOH:O	2.36	0.43
1:G:201:ILE:HD12	3:G:429:HOH:O	2.19	0.43
1:I:243:ILE:HG21	3:I:461:HOH:O	2.19	0.43
1:A:61:PHE:HB2	1:A:113:SER:HA	2.00	0.42
1:A:92:LEU:HD22	1:A:106:LEU:HD21	2.00	0.42
1:F:114:ILE:HA	1:F:118:LEU:HD11	2.00	0.42
1:G:79:PHE:O	1:G:102:ARG:NH2	2.52	0.42
1:I:177:GLY:HA3	1:I:178:LYS:HA	1.75	0.42
1:I:263:VAL:HG12	1:I:267:LYS:HE3	2.00	0.42
1:K:72:ASP:N	1:K:72:ASP:OD1	2.50	0.42
1:K:182:ARG:HB3	1:K:187:PHE:CZ	2.53	0.42
1:E:14:ARG:NH1	1:F:74:ASN:HD21	2.16	0.42
1:K:16:ASP:O	1:K:18:PRO:HD3	2.19	0.42
1:D:33:ASP:OD1	3:D:420:HOH:O	2.21	0.42
1:E:58:HIS:NE2	2:E:301:26T:H5	2.35	0.42
1:E:262:PRO:O	1:E:266:MET:HG3	2.19	0.42
1:G:258:GLN:CG	1:G:259:SER:N	2.83	0.42
1:H:218:CYS:HA	1:H:219:PRO:HD3	1.82	0.42
1:I:48:THR:HB	1:I:50:LYS:HE3	2.02	0.42
1:K:206:TYR:HB2	1:K:224:ILE:HD12	2.01	0.42
1:C:233:ARG:HB2	1:C:283:TYR:CE1	2.54	0.42
1:K:229:LYS:HE3	3:K:403:HOH:O	2.19	0.42
1:A:76:ALA:HA	1:A:79:PHE:CE2	2.53	0.42
1:A:256:ILE:HD13	1:A:266:MET:HG2	2.00	0.42
1:B:115:LEU:HD12	1:C:144:ILE:HG22	2.01	0.42
1:D:253:GLY:HA3	2:D:301:26T:O09	2.19	0.42
1:D:265:MET:O	1:D:268:ALA:HB3	2.20	0.42
1:I:106:LEU:HB3	1:I:125:LEU:HD21	2.01	0.42
1:C:269:VAL:O	1:C:272:VAL:HG12	2.19	0.42
1:D:58:HIS:CE1	2:D:301:26T:C05	2.99	0.42
1:D:262:PRO:O	1:D:265:MET:HG2	2.19	0.42
1:K:261:HIS:ND1	1:K:287:LEU:HD11	2.34	0.42
1:B:165:LYS:O	1:I:132:ARG:NH2	2.53	0.42
1:D:256:ILE:HD13	1:D:266:MET:HG3	2.02	0.42
1:D:273:VAL:HG23	1:D:274:HIS:N	2.35	0.42
1:E:204:THR:CG2	1:E:205:TYR:N	2.82	0.42
1:F:103:PRO:HB3	1:F:136:CYS:SG	2.60	0.42
1:D:250:VAL:HG12	1:D:252:MET:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:LEU:HG	3:I:458:HOH:O	2.19	0.42
1:I:229:LYS:HB2	1:I:258:GLN:OE1	2.20	0.42
1:A:53:MET:HA	1:A:84:VAL:HG13	2.02	0.42
1:B:73:ILE:HD13	1:I:17:GLN:OE1	2.20	0.42
1:B:204:THR:O	1:B:224:ILE:HA	2.20	0.42
1:B:271:ALA:HA	1:B:275:HIS:HB2	2.00	0.42
1:C:209:LYS:HA	1:C:209:LYS:HD2	1.83	0.42
1:C:233:ARG:HB2	1:C:283:TYR:HE1	1.84	0.42
1:D:283:TYR:HD1	1:D:283:TYR:HA	1.71	0.42
1:G:106:LEU:HD23	1:G:106:LEU:HA	1.89	0.42
1:H:211:PHE:HB3	1:H:245:GLN:HE21	1.83	0.42
1:K:265:MET:O	1:K:269:VAL:HG23	2.19	0.42
1:C:45:ASN:HA	1:C:46:PRO:HD3	1.94	0.42
1:G:176:VAL:HG21	1:G:182:ARG:CZ	2.50	0.42
1:H:26:LEU:HD21	1:H:44:PHE:CD2	2.54	0.42
1:A:131:VAL:CG2	1:A:166:VAL:HG11	2.50	0.41
1:A:260:ASP:OD1	1:A:260:ASP:N	2.48	0.41
1:C:22:ILE:HA	1:C:23:PRO:HD3	1.80	0.41
1:C:271:ALA:HB1	1:C:277:GLU:HG3	2.01	0.41
1:D:50:LYS:NZ	1:D:273:VAL:O	2.51	0.41
1:G:93:ARG:CZ	1:G:133:LEU:HD21	2.50	0.41
1:A:252:MET:SD	1:A:255:ASN:HB2	2.59	0.41
1:A:260:ASP:O	1:A:261:HIS:ND1	2.54	0.41
1:C:224:ILE:HD11	1:C:242:ALA:CB	2.50	0.41
1:D:133:LEU:CD2	1:G:34:TRP:HB3	2.49	0.41
1:D:256:ILE:CA	1:D:265:MET:SD	3.08	0.41
1:D:32:LEU:HB2	1:D:37:GLN:HG3	2.01	0.41
1:D:143:TYR:O	1:D:149:GLU:HB2	2.20	0.41
1:E:62:GLN:HA	1:E:114:ILE:HG12	2.02	0.41
1:E:149:GLU:O	1:E:153:ILE:HG13	2.21	0.41
1:H:236:LEU:HD12	1:H:283:TYR:CD2	2.55	0.41
1:H:236:LEU:HB2	1:H:283:TYR:CE2	2.56	0.41
1:H:281:ARG:HA	1:H:284:GLU:HB3	2.02	0.41
1:H:287:LEU:O	1:H:287:LEU:HG	2.20	0.41
1:K:177:GLY:HA3	1:K:180:MET:CG	2.48	0.41
1:A:173:VAL:HG22	1:A:203:ALA:HB3	2.02	0.41
1:C:178:LYS:HG3	1:C:178:LYS:O	2.20	0.41
1:G:11:LYS:HB3	1:G:13:PHE:CE1	2.56	0.41
1:G:100:THR:HG22	1:G:102:ARG:HB2	2.01	0.41
1:G:256:ILE:C	1:G:258:GLN:N	2.78	0.41
1:B:70:ARG:HH21	1:I:19:GLN:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:MET:HE2	1:B:266:MET:HB3	1.94	0.41
1:C:17:GLN:NE2	1:H:73:ILE:HD13	2.35	0.41
1:D:232:GLU:CD	1:D:259:SER:HB2	2.45	0.41
1:E:82:ALA:HB2	1:E:266:MET:HE1	2.01	0.41
1:G:60:TYR:HA	1:H:196:GLU:HG2	2.02	0.41
1:G:278:THR:HG21	1:G:281:ARG:CZ	2.50	0.41
1:D:107:ARG:HH21	1:D:141:GLN:NE2	2.18	0.41
1:E:55:ALA:HA	1:E:86:MET:HB3	2.02	0.41
1:I:83:ASP:O	1:I:103:PRO:HD2	2.21	0.41
1:C:143:TYR:CD1	1:C:175:GLY:HA3	2.55	0.41
1:H:84:VAL:HG11	1:H:105:VAL:HG23	2.03	0.41
1:I:187:PHE:CZ	1:I:205:TYR:HB2	2.55	0.41
1:E:53:MET:HG3	1:E:84:VAL:HG13	2.03	0.41
1:H:117:GLU:CD	1:H:119:SER:H	2.29	0.41
1:I:95:VAL:O	1:I:97:PRO:HD3	2.20	0.41
1:A:13:PHE:CE1	1:A:15:THR:HB	2.55	0.41
1:A:233:ARG:HA	1:A:283:TYR:CZ	2.56	0.41
1:A:256:ILE:HG21	1:A:266:MET:HE2	2.03	0.41
1:B:265:MET:O	1:B:269:VAL:HG23	2.20	0.41
1:D:13:PHE:CG	1:H:213:ARG:HG2	2.55	0.41
1:D:133:LEU:HA	1:G:35:GLY:HA3	2.02	0.41
1:D:144:ILE:HD13	1:D:193:ILE:HD12	2.03	0.41
1:E:19:GLN:NE2	1:F:95:VAL:HG12	2.36	0.41
1:F:184:GLN:HG3	1:F:210:GLY:O	2.21	0.41
1:G:176:VAL:HG21	1:G:182:ARG:NH1	2.36	0.41
1:H:145:GLY:N	1:H:149:GLU:OE1	2.37	0.41
1:H:203:ALA:HA	1:H:223:VAL:O	2.20	0.41
1:H:203:ALA:HB2	3:H:435:HOH:O	2.20	0.41
1:K:173:VAL:HG22	1:K:203:ALA:HB3	2.02	0.41
1:A:12:ASP:O	1:K:69:GLU:HG3	2.21	0.41
1:A:160:VAL:O	1:A:164:MET:HG2	2.21	0.41
1:D:171:MET:CB	1:D:201:ILE:HG23	2.50	0.41
1:F:212:GLU:CG	1:F:245:GLN:HB3	2.45	0.41
1:A:132:ARG:HA	1:K:166:VAL:O	2.22	0.40
1:C:58:HIS:HB2	1:C:68:LEU:HD22	2.04	0.40
1:D:107:ARG:HD2	1:D:107:ARG:HA	1.81	0.40
1:D:119:SER:HA	1:D:143:TYR:CZ	2.56	0.40
1:K:287:LEU:HD23	1:K:287:LEU:HA	1.58	0.40
1:A:14:ARG:NH1	1:K:74:ASN:OD1	2.54	0.40
1:B:23:PRO:O	3:B:443:HOH:O	2.22	0.40
1:B:42:ARG:HB3	1:B:103:PRO:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:PHE:CD1	1:D:56:PHE:N	2.90	0.40
1:E:71:ILE:HG23	1:E:75:ILE:CG2	2.51	0.40
1:I:287:LEU:C	1:I:289:GLU:N	2.79	0.40
3:A:427:HOH:O	1:K:70:ARG:NH2	2.53	0.40
1:B:58:HIS:HE2	2:B:301:26T:H5	1.86	0.40
1:B:252:MET:HE3	1:B:252:MET:HB2	1.83	0.40
1:E:47:LYS:HG3	1:E:48:THR:N	2.33	0.40
1:H:95:VAL:O	1:H:97:PRO:HD3	2.22	0.40
1:A:184:GLN:HE22	1:A:213:ARG:CB	2.34	0.40
1:D:13:PHE:CE1	1:G:69:GLU:HG2	2.56	0.40
1:D:48:THR:HG22	1:D:50:LYS:H	1.86	0.40
1:D:236:LEU:HD12	1:D:282:ALA:HB1	2.03	0.40
1:F:144:ILE:HG22	1:I:115:LEU:HD12	2.04	0.40
1:G:259:SER:HB3	1:G:261:HIS:H	1.86	0.40
1:G:280:ASP:OD1	1:G:280:ASP:N	2.54	0.40
1:I:265:MET:HB2	1:I:286:TYR:HE1	1.87	0.40
1:K:56:PHE:CD1	1:K:56:PHE:N	2.89	0.40
1:A:239:CYS:SG	1:A:252:MET:HE1	2.61	0.40
1:C:218:CYS:HA	1:C:219:PRO:HD3	1.78	0.40
1:D:39:ARG:NH1	1:D:167:GLY:O	2.55	0.40
1:D:78:LEU:HD11	1:D:262:PRO:C	2.47	0.40
1:E:206:TYR:CE2	1:E:208:GLU:HG2	2.56	0.40
1:I:270:GLN:HE21	1:I:270:GLN:HB2	1.75	0.40

All (2) 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:C:287:LEU:O	1:D:47:LYS:NZ[2_454]	2.12	0.08
3:C:401:HOH:O	3:I:403:HOH:O[1_455]	2.19	0.01

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	279/293 (95%)	267 (96%)	12 (4%)	0	100	100
1	B	279/293 (95%)	269 (96%)	9 (3%)	1 (0%)	30	49
1	C	279/293 (95%)	266 (95%)	11 (4%)	2 (1%)	18	34
1	D	279/293 (95%)	267 (96%)	8 (3%)	4 (1%)	9	17
1	E	279/293 (95%)	268 (96%)	10 (4%)	1 (0%)	30	49
1	F	278/293 (95%)	266 (96%)	11 (4%)	1 (0%)	30	49
1	G	279/293 (95%)	266 (95%)	11 (4%)	2 (1%)	18	34
1	H	279/293 (95%)	265 (95%)	11 (4%)	3 (1%)	11	22
1	I	279/293 (95%)	265 (95%)	10 (4%)	4 (1%)	9	17
1	K	279/293 (95%)	267 (96%)	12 (4%)	0	100	100
All	All	2789/2930 (95%)	2666 (96%)	105 (4%)	18 (1%)	21	38

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	LYS
1	D	178	LYS
1	D	286	TYR
1	E	178	LYS
1	F	178	LYS
1	G	287	LEU
1	G	288	SER
1	C	179	ASP
1	H	178	LYS
1	H	181	VAL
1	I	177	GLY
1	I	288	SER
1	C	284	GLU
1	H	179	ASP
1	D	254	ARG
1	I	174	THR
1	I	287	LEU
1	D	235	ALA

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	227/237 (96%)	219 (96%)	8 (4%)	32	58
1	B	227/237 (96%)	223 (98%)	4 (2%)	51	77
1	C	227/237 (96%)	224 (99%)	3 (1%)	61	82
1	D	227/237 (96%)	208 (92%)	19 (8%)	10	22
1	E	227/237 (96%)	218 (96%)	9 (4%)	28	54
1	F	226/237 (95%)	219 (97%)	7 (3%)	35	62
1	G	227/237 (96%)	213 (94%)	14 (6%)	16	34
1	H	227/237 (96%)	216 (95%)	11 (5%)	23	46
1	I	227/237 (96%)	218 (96%)	9 (4%)	28	54
1	K	227/237 (96%)	217 (96%)	10 (4%)	25	50
All	All	2269/2370 (96%)	2175 (96%)	94 (4%)	27	53

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	84	VAL
1	A	125	LEU
1	A	166	VAL
1	A	193	ILE
1	A	260	ASP
1	A	269	VAL
1	A	274	HIS
1	B	74	ASN
1	B	180	MET
1	B	284	GLU
1	B	285	LEU
1	C	20	LYS
1	C	73	ILE
1	C	75	ILE
1	D	11	LYS

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Mol	Chain	Res	Type
1	D	56	PHE
1	D	58	HIS
1	D	69	GLU
1	D	78	LEU
1	D	84	VAL
1	D	212	GLU
1	D	214	ILE
1	D	220	VAL
1	D	224	ILE
1	D	233	ARG
1	D	236	LEU
1	D	252	MET
1	D	255	ASN
1	D	263	VAL
1	D	265	MET
1	D	266	MET
1	D	270	GLN
1	D	283	TYR
1	E	17	GLN
1	E	47	LYS
1	E	84	VAL
1	E	142	VAL
1	E	166	VAL
1	E	185	ARG
1	E	204	THR
1	E	209	LYS
1	E	276	ASN
1	F	15	THR
1	F	84	VAL
1	F	86	MET
1	F	173	VAL
1	F	180	MET
1	F	182	ARG
1	F	252	MET
1	G	19	GLN
1	G	84	VAL
1	G	89	ARG
1	G	102	ARG
1	G	142	VAL
1	G	166	VAL
1	G	184	GLN
1	G	200	GLN

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Mol	Chain	Res	Type
1	G	207	VAL
1	G	213	ARG
1	G	215	VAL
1	G	252	MET
1	G	270	GLN
1	G	286	TYR
1	H	20	LYS
1	H	66	THR
1	H	178	LYS
1	H	184	GLN
1	H	185	ARG
1	H	192	ARG
1	H	212	GLU
1	H	267	LYS
1	H	270	GLN
1	H	281	ARG
1	H	283	TYR
1	I	11	LYS
1	I	74	ASN
1	I	81	HIS
1	I	166	VAL
1	I	178	LYS
1	I	209	LYS
1	I	233	ARG
1	I	250	VAL
1	I	281	ARG
1	K	11	LYS
1	K	47	LYS
1	K	50	LYS
1	K	213	ARG
1	K	228	LYS
1	K	234	GLU
1	K	254	ARG
1	K	276	ASN
1	K	285	LEU
1	K	287	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	184	GLN

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Mol	Chain	Res	Type
1	B	74	ASN
1	B	134	ASN
1	C	17	GLN
1	C	81	HIS
1	C	158	GLN
1	D	74	ASN
1	D	255	ASN
1	E	101	ASN
1	E	151	GLN
1	E	258	GLN
1	F	151	GLN
1	F	276	ASN
1	G	58	HIS
1	G	81	HIS
1	G	151	GLN
1	G	200	GLN
1	G	245	GLN
1	G	270	GLN
1	G	275	HIS
1	I	74	ASN
1	I	151	GLN
1	K	245	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	26T	C	301	-	10,12,12	4.36	3 (30%)	9,17,17	2.08	4 (44%)
2	26T	A	301	-	10,12,12	4.48	3 (30%)	9,17,17	1.97	4 (44%)
2	26T	G	301	-	10,12,12	4.44	3 (30%)	9,17,17	1.97	4 (44%)
2	26T	I	301	-	10,12,12	4.49	3 (30%)	9,17,17	2.04	4 (44%)
2	26T	H	301	-	10,12,12	4.52	3 (30%)	9,17,17	2.02	4 (44%)
2	26T	K	301	-	10,12,12	4.47	3 (30%)	9,17,17	2.04	4 (44%)
2	26T	E	301	-	10,12,12	4.45	3 (30%)	9,17,17	1.98	2 (22%)
2	26T	D	301	-	10,12,12	4.50	3 (30%)	9,17,17	2.07	4 (44%)
2	26T	F	301	-	10,12,12	4.44	3 (30%)	9,17,17	2.17	4 (44%)
2	26T	B	301	-	10,12,12	4.42	3 (30%)	9,17,17	2.02	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	26T	C	301	-	-	9/14/14/14	-
2	26T	A	301	-	-	6/14/14/14	-
2	26T	G	301	-	-	8/14/14/14	-
2	26T	I	301	-	-	5/14/14/14	-
2	26T	H	301	-	-	8/14/14/14	-
2	26T	K	301	-	-	9/14/14/14	-
2	26T	E	301	-	-	7/14/14/14	-
2	26T	D	301	-	-	7/14/14/14	-
2	26T	F	301	-	-	5/14/14/14	-
2	26T	B	301	-	-	6/14/14/14	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	26T	O06-C05	-11.16	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	26T	O06-C05	-11.00	1.32	1.43
2	I	301	26T	O06-C05	-10.48	1.32	1.43
2	K	301	26T	O06-C05	-10.41	1.33	1.43
2	H	301	26T	O06-C05	-10.25	1.33	1.43
2	B	301	26T	O06-C05	-10.11	1.33	1.43
2	A	301	26T	O06-C05	-9.98	1.33	1.43
2	E	301	26T	O06-C05	-9.87	1.33	1.43
2	C	301	26T	O06-C05	-9.81	1.33	1.43
2	G	301	26T	P07-O06	9.35	1.89	1.60
2	G	301	26T	O06-C05	-9.28	1.34	1.43
2	H	301	26T	P07-O06	8.96	1.88	1.60
2	A	301	26T	P07-O06	8.96	1.88	1.60
2	B	301	26T	P07-O06	8.84	1.88	1.60
2	E	301	26T	P07-O06	8.79	1.88	1.60
2	K	301	26T	P07-O06	8.62	1.87	1.60
2	I	301	26T	P07-O06	8.60	1.87	1.60
2	D	301	26T	P07-O06	8.52	1.87	1.60
2	C	301	26T	P07-O06	8.35	1.86	1.60
2	F	301	26T	P07-O06	7.79	1.84	1.60
2	G	301	26T	C05-C04	4.36	1.58	1.51
2	C	301	26T	C05-C04	4.27	1.57	1.51
2	E	301	26T	C05-C04	4.25	1.57	1.51
2	A	301	26T	C05-C04	3.87	1.57	1.51
2	H	301	26T	C05-C04	3.75	1.57	1.51
2	I	301	26T	C05-C04	3.66	1.57	1.51
2	K	301	26T	C05-C04	3.38	1.56	1.51
2	B	301	26T	C05-C04	3.21	1.56	1.51
2	F	301	26T	C05-C04	2.75	1.55	1.51
2	D	301	26T	C05-C04	2.14	1.54	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	26T	O13-C02-C01	-3.26	115.41	121.17
2	F	301	26T	O13-C02-C01	-3.25	115.42	121.17
2	C	301	26T	O13-C02-C01	-3.19	115.54	121.17
2	G	301	26T	O13-C02-C01	-3.18	115.56	121.17
2	H	301	26T	O13-C02-C01	-3.15	115.61	121.17
2	B	301	26T	O13-C02-C01	-3.14	115.63	121.17
2	I	301	26T	O13-C02-C01	-3.04	115.80	121.17
2	K	301	26T	O13-C02-C01	-3.04	115.80	121.17
2	A	301	26T	O13-C02-C01	-3.03	115.82	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	26T	O08-P07-O06	-3.00	98.85	106.67
2	E	301	26T	O13-C02-C01	-2.91	116.03	121.17
2	K	301	26T	O08-P07-O06	-2.89	99.12	106.67
2	B	301	26T	O08-P07-O06	-2.88	99.16	106.67
2	C	301	26T	O09-P07-O06	-2.84	99.25	106.67
2	I	301	26T	O08-P07-O06	-2.79	99.38	106.67
2	A	301	26T	O08-P07-O06	-2.72	99.57	106.67
2	E	301	26T	O08-P07-O06	-2.71	99.60	106.67
2	H	301	26T	O06-P07-O10	-2.65	99.28	106.44
2	C	301	26T	O08-P07-O06	-2.64	99.80	106.67
2	G	301	26T	O08-P07-O06	-2.59	99.90	106.67
2	D	301	26T	O06-P07-O10	-2.56	99.53	106.44
2	D	301	26T	O09-P07-O08	2.49	117.12	107.80
2	F	301	26T	O09-P07-O08	2.48	117.10	107.80
2	H	301	26T	O08-P07-O06	-2.45	100.29	106.67
2	G	301	26T	O09-P07-O08	2.44	116.95	107.80
2	H	301	26T	O09-P07-O08	2.43	116.93	107.80
2	I	301	26T	O06-P07-O10	-2.41	99.93	106.44
2	F	301	26T	O06-P07-O10	-2.40	99.96	106.44
2	D	301	26T	O08-P07-O06	-2.39	100.44	106.67
2	I	301	26T	O09-P07-O08	2.34	116.58	107.80
2	G	301	26T	O06-P07-O10	-2.33	100.14	106.44
2	K	301	26T	O09-P07-O06	-2.29	100.69	106.67
2	A	301	26T	O06-P07-O10	-2.25	100.37	106.44
2	A	301	26T	O09-P07-O08	2.23	116.16	107.80
2	B	301	26T	O09-P07-O06	-2.22	100.88	106.67
2	C	301	26T	O09-P07-O08	2.16	115.92	107.80
2	K	301	26T	O09-P07-O08	2.05	115.49	107.80
2	B	301	26T	O09-P07-O08	2.03	115.42	107.80

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	26T	C01-C02-C03-O12
2	A	301	26T	O13-C02-C03-O12
2	A	301	26T	O12-C03-C04-O11
2	A	301	26T	C05-O06-P07-O08
2	B	301	26T	O12-C03-C04-O11
2	B	301	26T	C03-C04-C05-O06
2	B	301	26T	O11-C04-C05-O06
2	B	301	26T	C05-O06-P07-O08

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Mol	Chain	Res	Type	Atoms
2	B	301	26T	C05-O06-P07-O09
2	C	301	26T	C01-C02-C03-O12
2	C	301	26T	O13-C02-C03-O12
2	C	301	26T	O12-C03-C04-O11
2	C	301	26T	C03-C04-C05-O06
2	C	301	26T	O11-C04-C05-O06
2	C	301	26T	C05-O06-P07-O08
2	C	301	26T	C05-O06-P07-O09
2	C	301	26T	C05-O06-P07-O10
2	D	301	26T	C01-C02-C03-O12
2	D	301	26T	O13-C02-C03-O12
2	D	301	26T	O12-C03-C04-O11
2	D	301	26T	C03-C04-C05-O06
2	D	301	26T	O11-C04-C05-O06
2	E	301	26T	C02-C03-C04-O11
2	E	301	26T	C05-O06-P07-O08
2	E	301	26T	C05-O06-P07-O09
2	E	301	26T	C05-O06-P07-O10
2	F	301	26T	O12-C03-C04-O11
2	G	301	26T	C01-C02-C03-O12
2	G	301	26T	O13-C02-C03-O12
2	G	301	26T	O12-C03-C04-O11
2	G	301	26T	C04-C05-O06-P07
2	G	301	26T	C05-O06-P07-O08
2	G	301	26T	C05-O06-P07-O09
2	H	301	26T	O13-C02-C03-O12
2	H	301	26T	O12-C03-C04-O11
2	H	301	26T	C03-C04-C05-O06
2	H	301	26T	O11-C04-C05-O06
2	H	301	26T	C05-O06-P07-O08
2	H	301	26T	C05-O06-P07-O09
2	I	301	26T	O13-C02-C03-O12
2	I	301	26T	O12-C03-C04-O11
2	I	301	26T	C05-O06-P07-O08
2	I	301	26T	C05-O06-P07-O09
2	K	301	26T	C01-C02-C03-O12
2	K	301	26T	O13-C02-C03-O12
2	K	301	26T	C02-C03-C04-C05
2	K	301	26T	C02-C03-C04-O11
2	K	301	26T	O12-C03-C04-O11
2	K	301	26T	C03-C04-C05-O06
2	K	301	26T	O11-C04-C05-O06

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Mol	Chain	Res	Type	Atoms
2	A	301	26T	C05-O06-P07-O10
2	B	301	26T	C05-O06-P07-O10
2	H	301	26T	C05-O06-P07-O10
2	I	301	26T	C05-O06-P07-O10
2	D	301	26T	O12-C03-C04-C05
2	F	301	26T	O12-C03-C04-C05
2	K	301	26T	O12-C03-C04-C05
2	A	301	26T	C05-O06-P07-O09
2	F	301	26T	C01-C02-C03-O12
2	H	301	26T	C01-C02-C03-O12
2	C	301	26T	C02-C03-C04-O11
2	D	301	26T	C02-C03-C04-O11
2	G	301	26T	C02-C03-C04-O11
2	G	301	26T	C05-O06-P07-O10
2	E	301	26T	C04-C05-O06-P07
2	F	301	26T	C03-C04-C05-O06
2	K	301	26T	C05-O06-P07-O09
2	E	301	26T	O12-C03-C04-O11
2	F	301	26T	O13-C02-C03-O12
2	E	301	26T	C01-C02-C03-O12

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	26T	1	0
2	G	301	26T	2	0
2	I	301	26T	3	0
2	H	301	26T	3	0
2	K	301	26T	1	0
2	E	301	26T	2	0
2	D	301	26T	4	0
2	F	301	26T	1	0
2	B	301	26T	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	281/293 (95%)	-1.10	0 100 100	31, 50, 104, 156	0
1	B	281/293 (95%)	-1.39	0 100 100	19, 35, 56, 79	0
1	C	281/293 (95%)	-1.11	0 100 100	31, 49, 85, 145	0
1	D	281/293 (95%)	-0.82	0 100 100	37, 61, 113, 137	0
1	E	281/293 (95%)	-1.33	0 100 100	18, 37, 71, 124	0
1	F	280/293 (95%)	-1.43	0 100 100	19, 33, 53, 99	0
1	G	281/293 (95%)	-0.92	0 100 100	33, 58, 109, 201	0
1	H	281/293 (95%)	-1.07	0 100 100	30, 51, 90, 107	0
1	I	281/293 (95%)	-1.32	0 100 100	20, 37, 77, 147	0
1	K	281/293 (95%)	-1.19	0 100 100	28, 48, 88, 119	0
All	All	2809/2930 (95%)	-1.17	0 100 100	18, 45, 92, 201	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	26T	D	301	13/13	0.98	0.05	49,66,69,72	0
2	26T	K	301	13/13	0.98	0.05	47,58,72,73	0
2	26T	C	301	13/13	0.99	0.03	31,40,93,93	0
2	26T	A	301	13/13	0.99	0.04	50,55,86,86	0
2	26T	E	301	13/13	0.99	0.04	43,49,72,72	0
2	26T	F	301	13/13	0.99	0.04	37,63,67,69	0
2	26T	G	301	13/13	0.99	0.04	45,60,90,91	0
2	26T	H	301	13/13	0.99	0.04	53,58,67,68	0
2	26T	I	301	13/13	0.99	0.05	40,55,69,69	0
2	26T	B	301	13/13	0.99	0.05	39,46,55,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.