



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:30 AM UTC

PDB ID : 4XSX / pdb_00004xsx
Title : Crystal structure of CBR 703 bound to Escherichia coli RNA polymerase holoenzyme
Authors : Bae, B.; Darst, S.A.
Deposited on : 2015-01-22
Resolution : 3.71 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

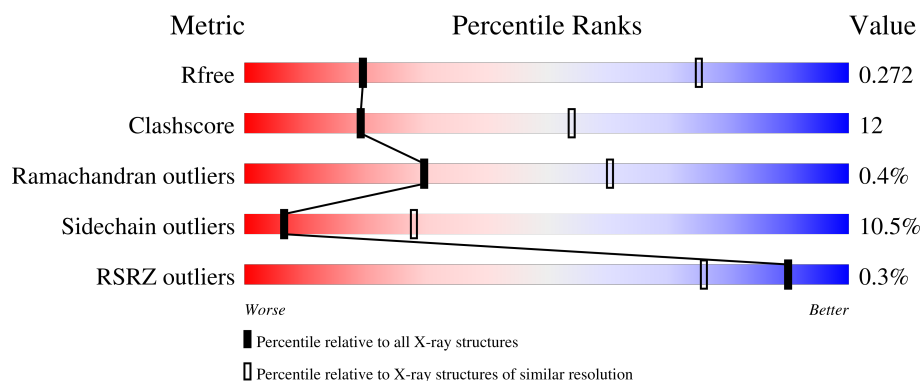
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	239	
1	B	239	
1	G	239	
1	H	239	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	 67%29%•
3	D	1407	 53%25%•17%
3	J	1407	 56%27%•12%
4	E	91	 74%20%••
4	K	91	 65%20%•13%
5	F	522	 60%26%•10%
5	L	522	 57%29%•10%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55722 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	B	220	Total	C	N	O	S	0	0	0
			1687	1053	298	330	6			
1	G	228	Total	C	N	O	S	0	0	0
			1750	1088	312	344	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	GLU	-	expression tag	UNP A7ZSI4
A	236	VAL	-	expression tag	UNP A7ZSI4
A	237	LEU	-	expression tag	UNP A7ZSI4
A	238	PHE	-	expression tag	UNP A7ZSI4
A	239	GLN	-	expression tag	UNP A7ZSI4
B	235	GLU	-	expression tag	UNP A7ZSI4
B	236	VAL	-	expression tag	UNP A7ZSI4
B	237	LEU	-	expression tag	UNP A7ZSI4
B	238	PHE	-	expression tag	UNP A7ZSI4
B	239	GLN	-	expression tag	UNP A7ZSI4
G	235	GLU	-	expression tag	UNP A7ZSI4
G	236	VAL	-	expression tag	UNP A7ZSI4
G	237	LEU	-	expression tag	UNP A7ZSI4
G	238	PHE	-	expression tag	UNP A7ZSI4
G	239	GLN	-	expression tag	UNP A7ZSI4
H	235	GLU	-	expression tag	UNP A7ZSI4
H	236	VAL	-	expression tag	UNP A7ZSI4
H	237	LEU	-	expression tag	UNP A7ZSI4
H	238	PHE	-	expression tag	UNP A7ZSI4
H	239	GLN	-	expression tag	UNP A7ZSI4

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1236	Total	C	N	O	S	0	0	0
			9638	6058	1726	1807	47			

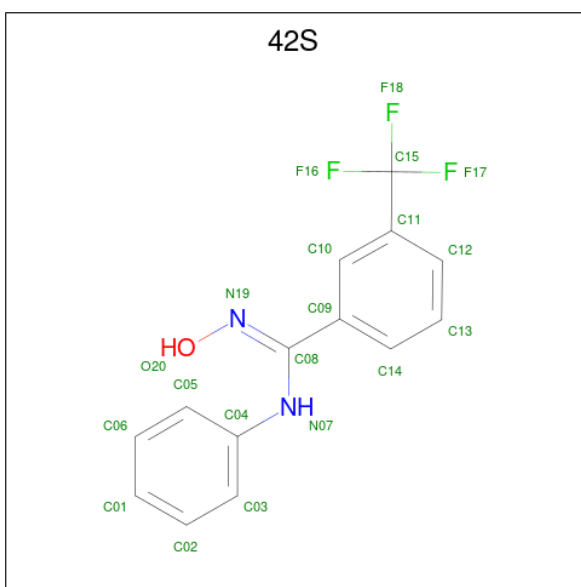
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	470	Total	C	N	O	S	0	0	0
			3822	2394	680	725	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is N'-hydroxy-N-phenyl-3-(trifluoromethyl)benzenecarboximidamide (CCD ID: 42S) (formula: C₁₄H₁₁F₃N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	F	N	O	0	0
			20	14	3	2	1		
6	I	1	Total	C	F	N	O	0	0
			20	14	3	2	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	J	1	Total	Mg	0	0
			1	1		

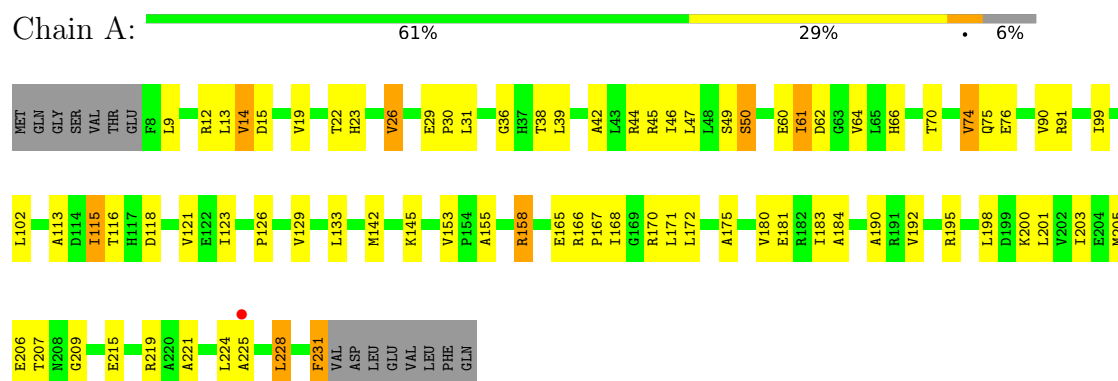
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	J	2	Total	Zn	0	0
			2	2		

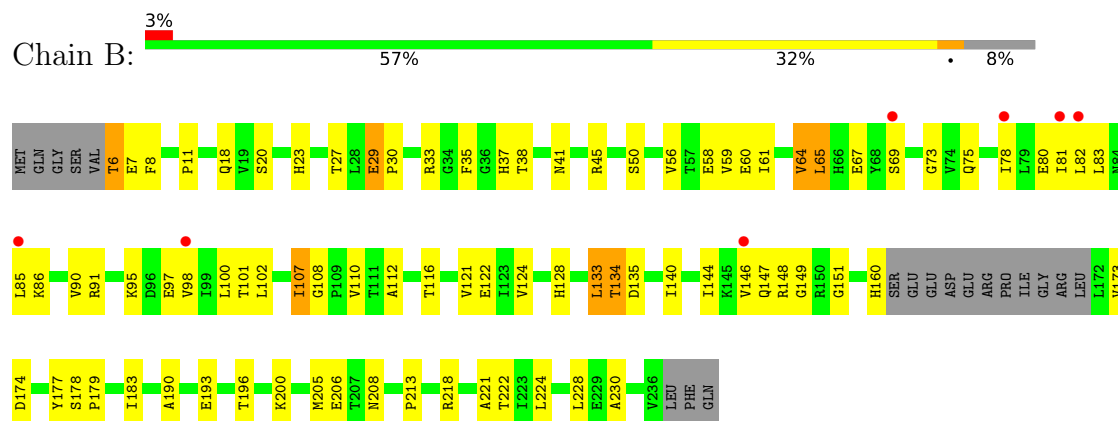
3 Residue-property plots [i](#)

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.

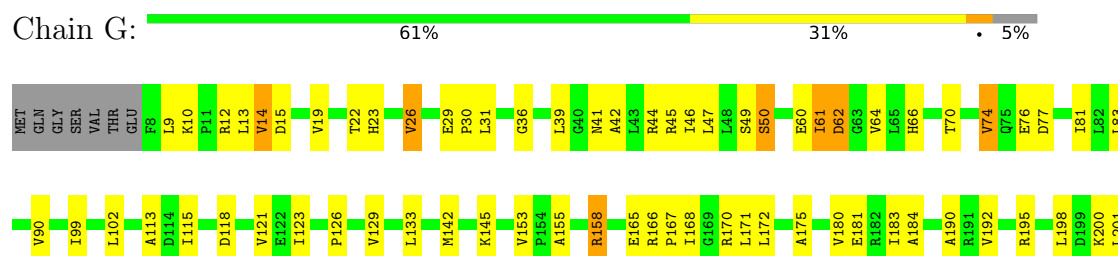
• Molecule 1: DNA-directed RNA polymerase subunit alpha



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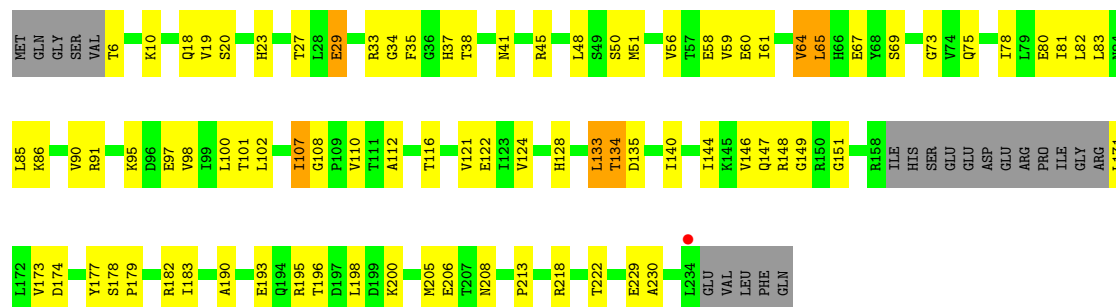
• Molecule 1: DNA-directed RNA polymerase subunit alpha





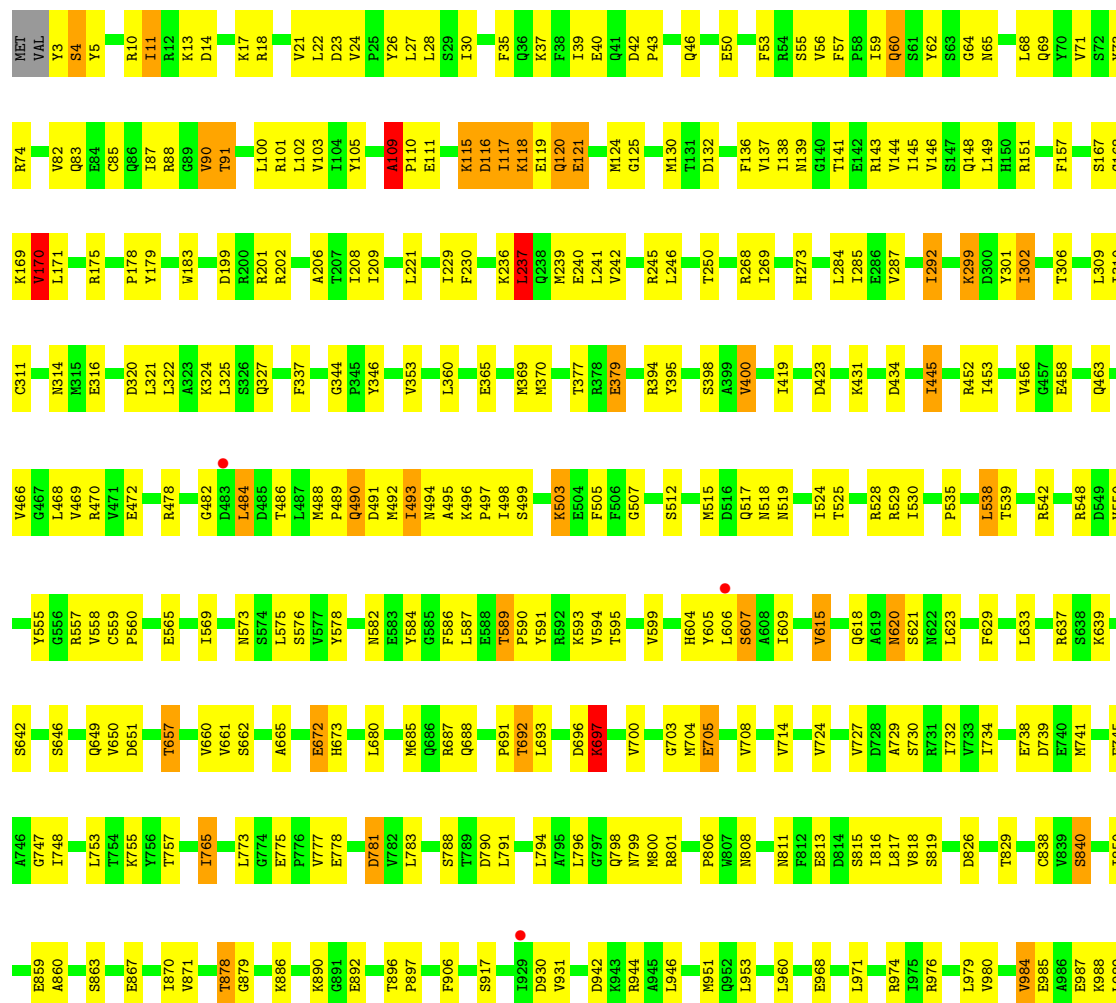
• Molecule 1: DNA-directed RNA polymerase subunit alpha

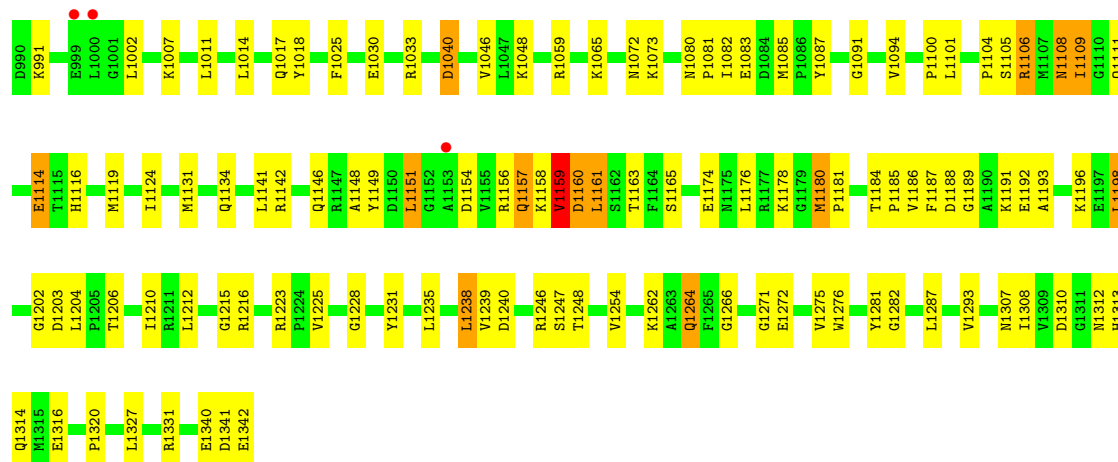
Chain H: 55% 33% 9%



• Molecule 2: DNA-directed RNA polymerase subunit beta

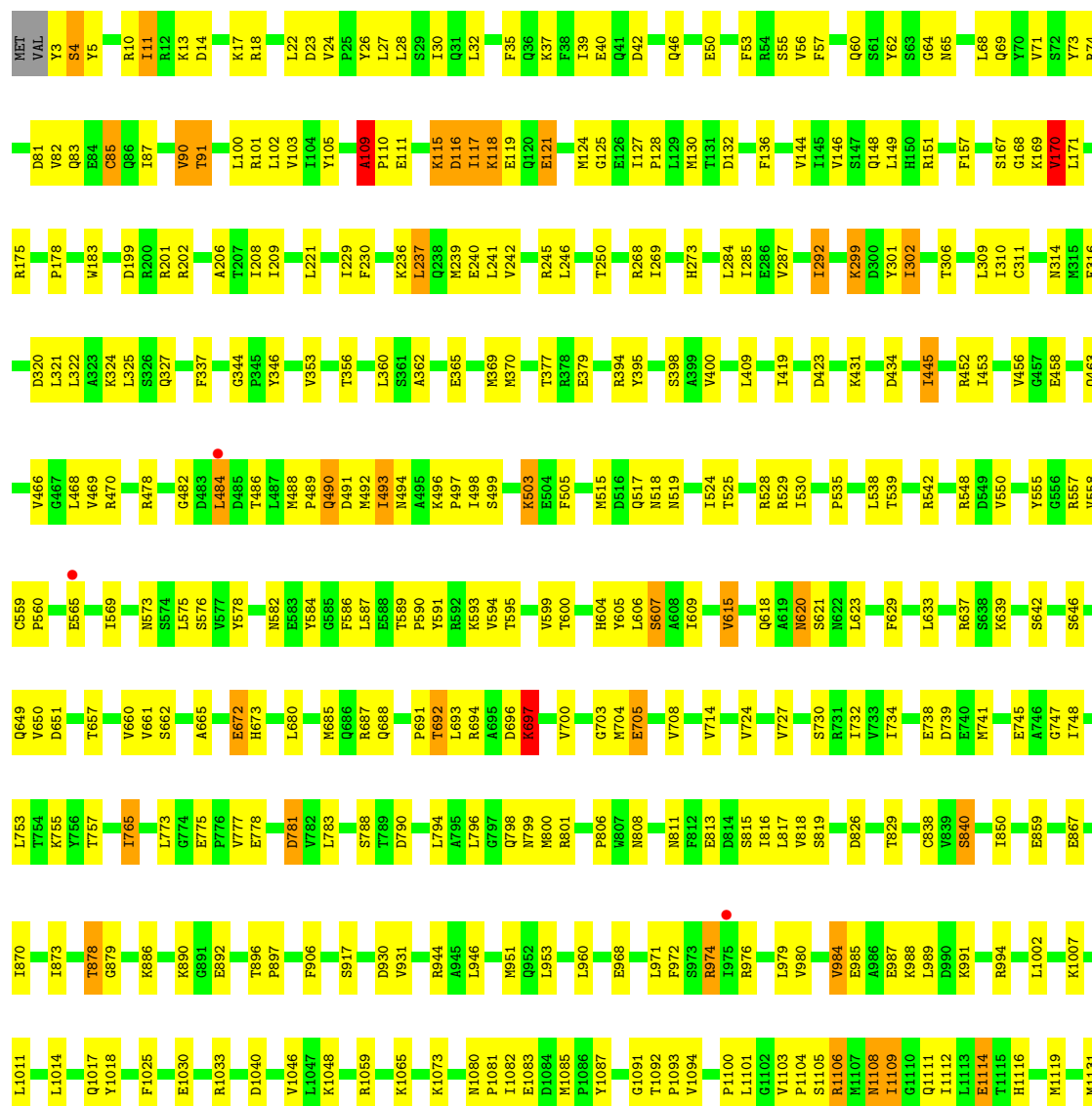
Chain C: 67% 29% 4%

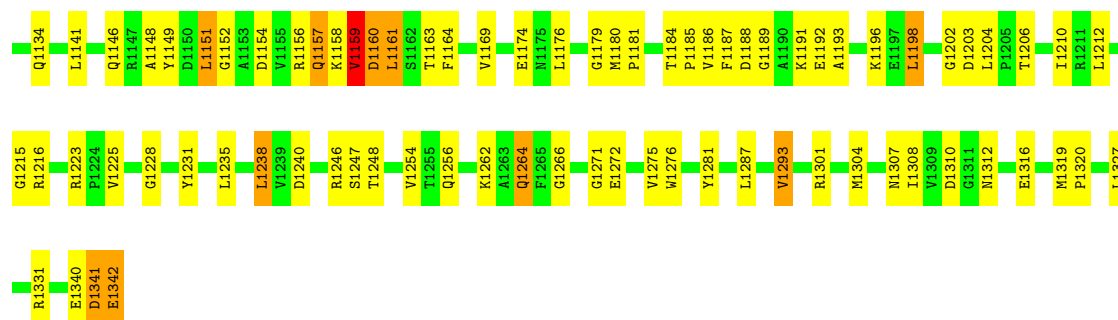




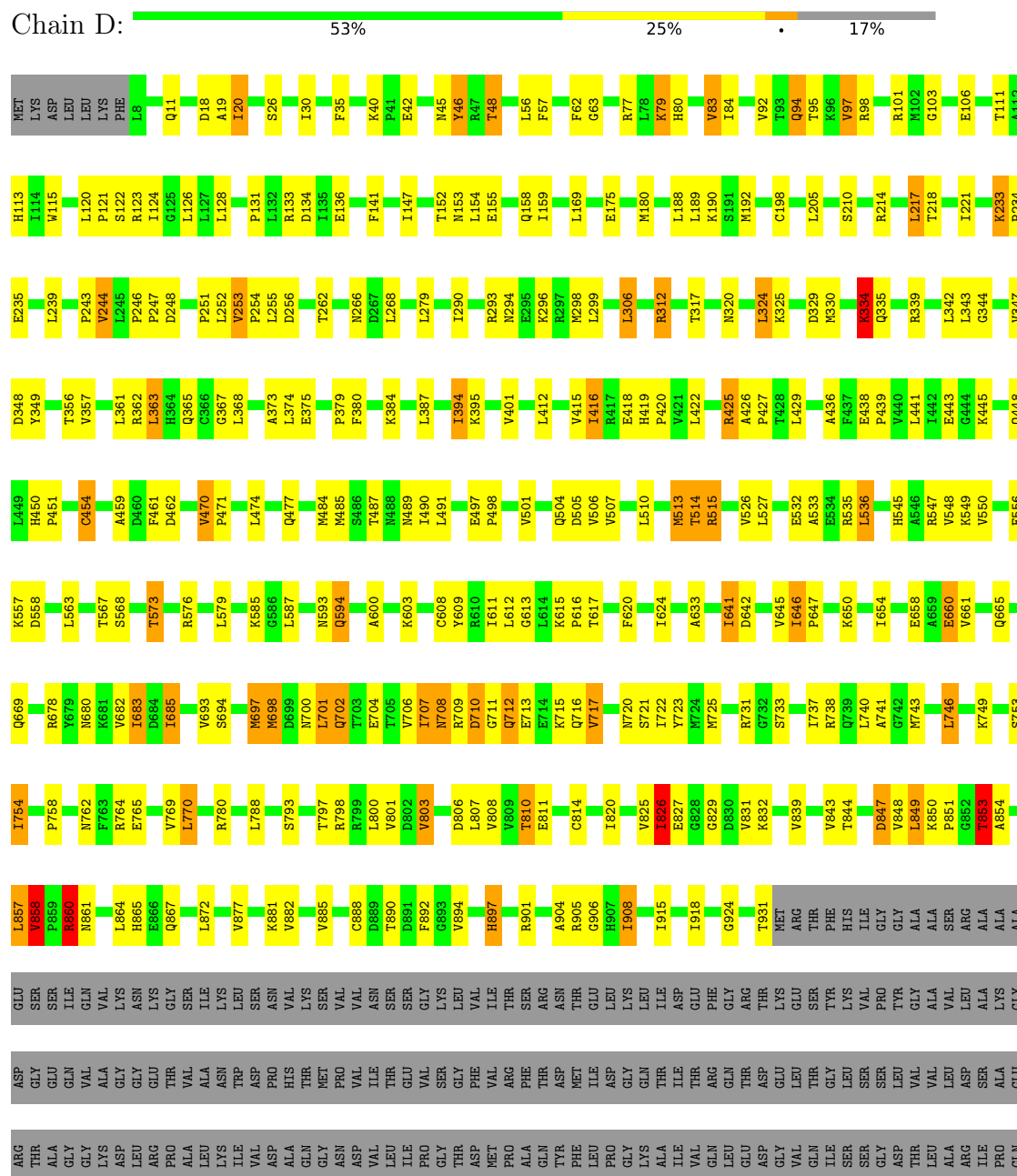
• Molecule 2: DNA-directed RNA polymerase subunit beta

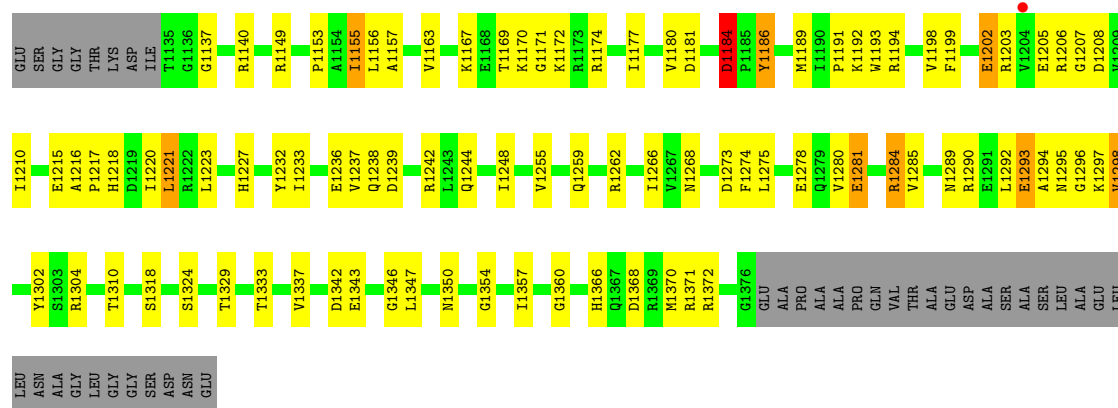
Chain I: 67% 29% •





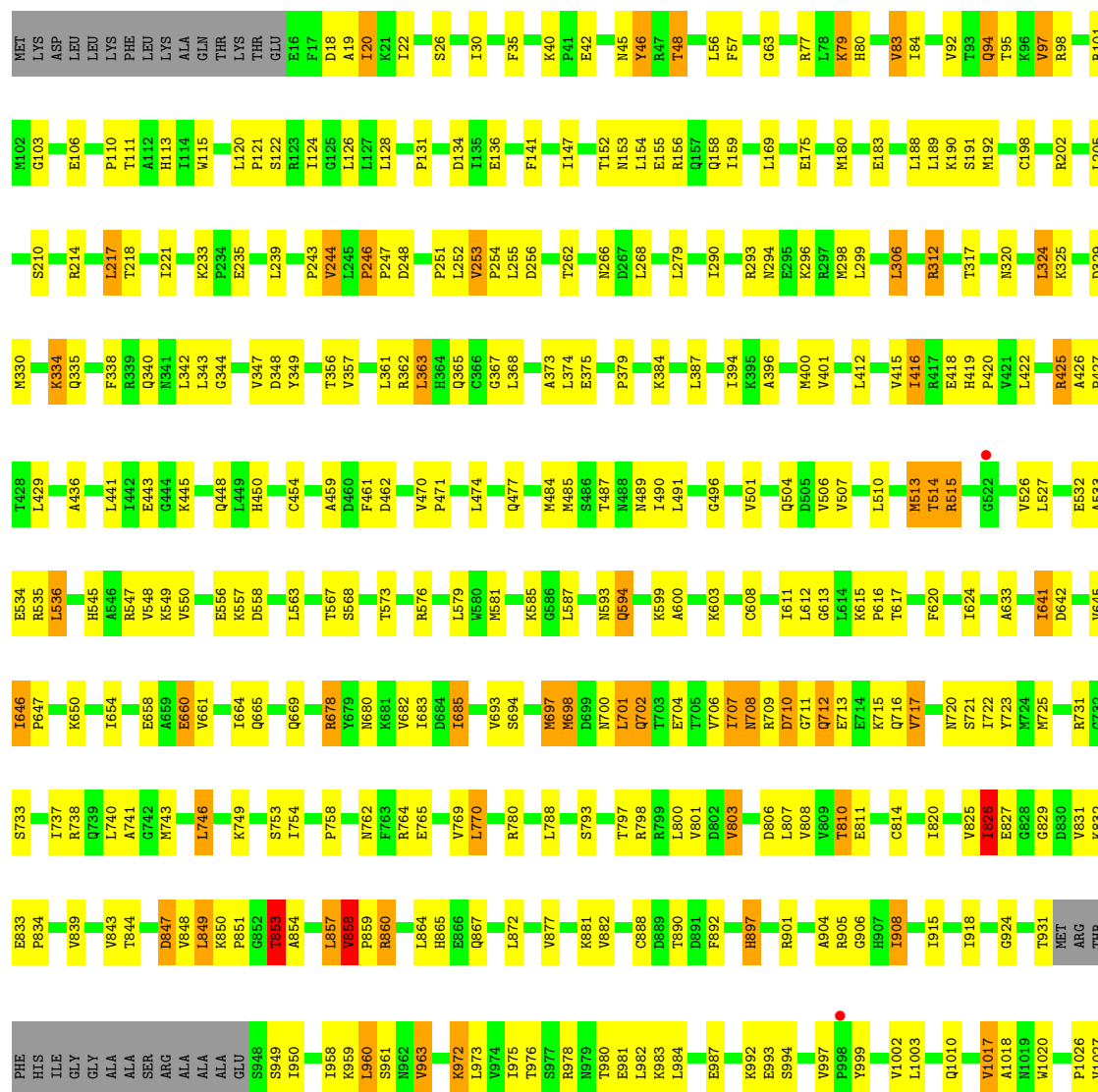
- Molecule 3: DNA-directed RNA polymerase subunit beta'

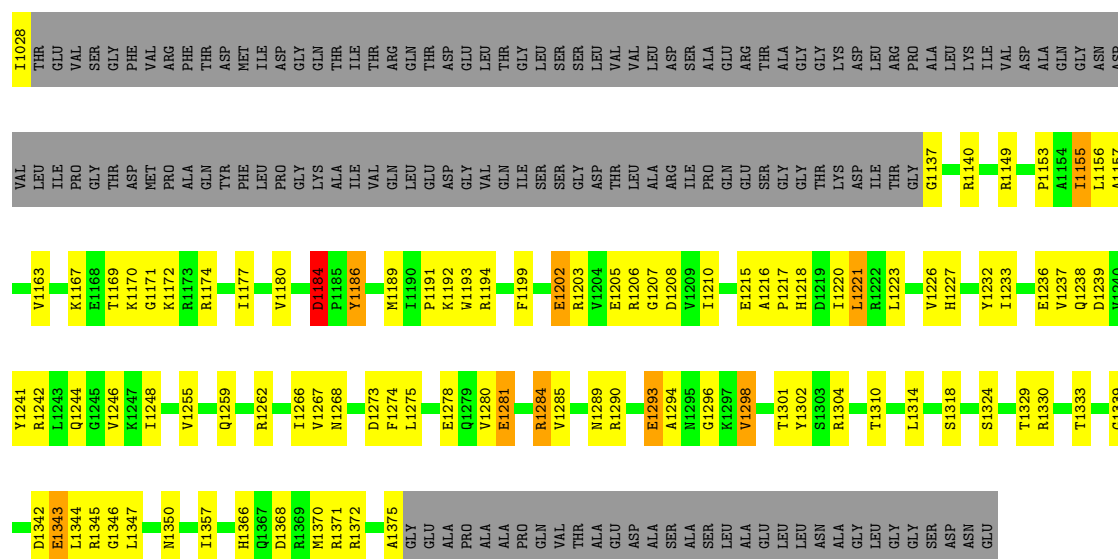




• Molecule 3: DNA-directed RNA polymerase subunit beta'

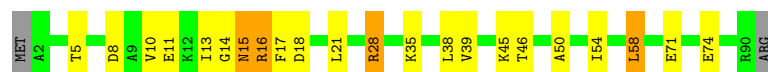
Chain J: 56% 27% 12%





- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 74% 20%



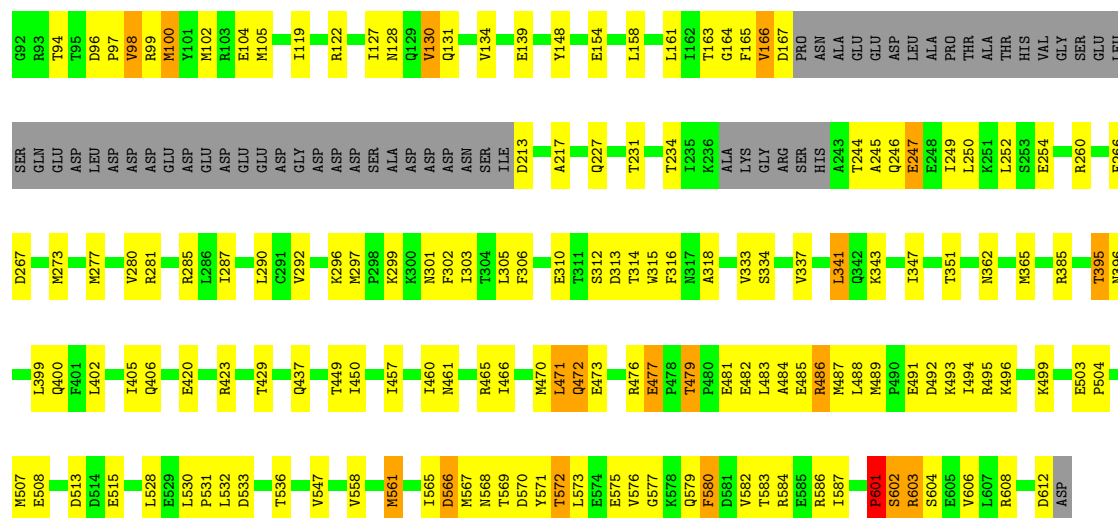
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 65% 20% 13%

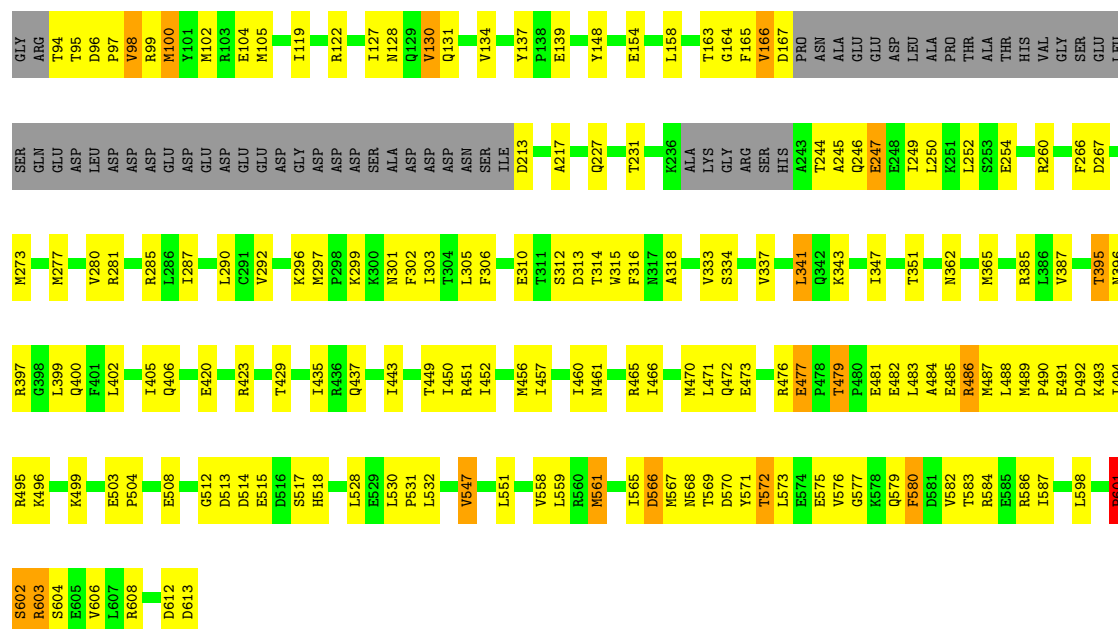


- Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 60% 26% 10%



Chain L: 57% 29% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.03Å 206.91Å 310.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.71 40.00 – 3.71	Depositor EDS
% Data completeness (in resolution range)	98.9 (40.00-3.71) 98.7 (40.00-3.71)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.273 0.228 , 0.272	Depositor DCC
R_{free} test set	6332 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	142.3	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55722	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: MG, ZN, 42S

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	0.36	0/1751	0.87	2/2373 (0.1%)
1	B	0.41	0/1707	0.88	3/2314 (0.1%)
1	G	0.38	0/1771	0.90	3/2401 (0.1%)
1	H	0.39	0/1686	0.87	3/2285 (0.1%)
2	C	0.38	1/10739 (0.0%)	0.86	21/14489 (0.1%)
2	I	0.37	0/10735	0.84	18/14484 (0.1%)
3	D	0.37	0/9246	0.87	25/12478 (0.2%)
3	J	0.37	0/9785	0.87	30/13206 (0.2%)
4	E	0.38	0/693	0.91	2/935 (0.2%)
4	K	0.40	0/629	0.88	0/847
5	F	0.39	0/3873	0.87	8/5206 (0.2%)
5	L	0.40	0/3872	0.88	8/5205 (0.2%)
All	All	0.38	1/56487 (0.0%)	0.86	123/76223 (0.2%)

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
2	C	0	1
2	I	0	1
3	D	0	2
3	J	0	2
5	F	0	1
5	L	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	512	SER	CA-C	-5.12	1.46	1.52

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	109	ALA	CA-C-N	14.28	135.21	119.93
2	C	109	ALA	C-N-CA	14.28	135.21	119.93
1	G	232	VAL	N-CA-C	9.86	123.85	108.87
3	J	858	VAL	CA-C-N	8.55	130.53	119.84
3	J	858	VAL	C-N-CA	8.55	130.53	119.84
5	F	602	SER	N-CA-C	-8.46	92.78	110.80
3	D	858	VAL	CA-C-N	8.40	130.34	119.84
3	D	858	VAL	C-N-CA	8.40	130.34	119.84
5	L	166	VAL	N-CA-C	-8.28	97.75	108.93
5	F	166	VAL	N-CA-C	-8.26	97.77	108.93
5	L	602	SER	N-CA-C	-8.19	93.35	110.80
2	C	747	GLY	N-CA-C	7.47	119.86	110.96
3	D	853	THR	N-CA-C	7.47	118.12	108.34
3	D	339	ARG	N-CA-C	7.24	120.75	112.57
2	C	236	LYS	N-CA-C	7.22	119.36	110.91
2	I	747	GLY	N-CA-C	7.20	119.53	110.96
2	I	236	LYS	N-CA-C	7.19	119.32	110.91
3	J	853	THR	N-CA-C	7.15	117.70	108.34
2	I	1157	GLN	N-CA-C	6.74	118.63	111.28
2	C	1157	GLN	N-CA-C	6.68	118.56	111.28
3	D	253	VAL	CA-C-N	6.62	126.58	120.03
3	D	253	VAL	C-N-CA	6.62	126.58	120.03
3	D	334	LYS	CB-CG-CD	6.60	126.48	111.30
3	J	253	VAL	CA-C-N	6.56	126.53	120.03
3	J	253	VAL	C-N-CA	6.56	126.53	120.03
3	J	334	LYS	CB-CG-CD	6.54	126.34	111.30
3	J	1184	ASP	N-CA-C	6.32	122.29	113.57
2	C	512	SER	CA-C-N	-6.29	112.03	122.21
2	C	512	SER	C-N-CA	-6.29	112.03	122.21
3	J	334	LYS	N-CA-C	6.22	116.22	108.19
2	I	1159	VAL	N-CA-C	6.22	122.28	109.34
5	F	601	PRO	N-CA-C	6.21	120.25	110.50
3	D	1184	ASP	N-CA-C	6.13	122.03	113.57
2	C	1159	VAL	N-CA-C	6.13	122.09	109.34
5	L	601	PRO	N-CA-C	6.02	119.96	110.50
2	I	697	LYS	CA-C-N	-6.02	113.58	119.90
2	I	697	LYS	C-N-CA	-6.02	113.58	119.90
2	I	398	SER	CB-CA-C	-6.00	108.65	115.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	398	SER	CB-CA-C	-5.96	108.69	115.79
3	J	233	LYS	CA-C-N	5.94	126.10	119.32
3	J	233	LYS	C-N-CA	5.94	126.10	119.32
5	L	163	THR	N-CA-C	-5.94	105.89	113.02
3	D	515	ARG	N-CA-C	-5.86	99.83	108.79
5	F	163	THR	N-CA-C	-5.84	106.01	113.02
1	B	108	GLY	CA-C-N	5.83	125.83	119.89
1	B	108	GLY	C-N-CA	5.83	125.83	119.89
3	D	40	LYS	CA-C-N	5.83	125.93	119.87
3	D	40	LYS	C-N-CA	5.83	125.93	119.87
3	J	515	ARG	N-CA-C	-5.81	99.90	108.79
2	C	237	LEU	N-CA-C	5.79	123.12	110.80
2	I	237	LEU	N-CA-C	5.77	123.10	110.80
3	D	713	GLU	N-CA-C	5.77	116.70	108.74
3	J	713	GLU	N-CA-C	5.75	116.67	108.74
5	L	213	ASP	CA-C-N	5.73	125.85	119.32
5	L	213	ASP	C-N-CA	5.73	125.85	119.32
3	J	40	LYS	CA-C-N	5.72	125.82	119.87
3	J	40	LYS	C-N-CA	5.72	125.82	119.87
1	H	108	GLY	CA-C-N	5.70	125.70	119.89
1	H	108	GLY	C-N-CA	5.70	125.70	119.89
3	D	233	LYS	CA-C-N	5.66	125.77	119.32
3	D	233	LYS	C-N-CA	5.66	125.77	119.32
4	E	14	GLY	N-CA-C	5.65	119.06	112.50
2	C	1235	LEU	CA-C-N	-5.61	114.47	122.77
2	C	1235	LEU	C-N-CA	-5.61	114.47	122.77
2	C	573	ASN	CB-CA-C	-5.59	108.51	116.34
2	I	1235	LEU	CA-C-N	-5.59	114.50	122.77
2	I	1235	LEU	C-N-CA	-5.59	114.50	122.77
1	A	192	VAL	N-CA-C	-5.58	101.84	109.55
5	F	213	ASP	CA-C-N	5.57	125.67	119.32
5	F	213	ASP	C-N-CA	5.57	125.67	119.32
2	I	573	ASN	CB-CA-C	-5.55	108.57	116.34
3	D	860	ARG	CB-CA-C	-5.54	110.20	116.63
2	C	1239	VAL	CA-C-N	-5.54	114.15	122.24
2	C	1239	VAL	C-N-CA	-5.54	114.15	122.24
3	D	48	THR	N-CA-C	-5.49	101.51	109.59
1	B	20	SER	CB-CA-C	-5.49	110.26	116.63
3	J	860	ARG	CB-CA-C	-5.48	110.27	116.63
3	J	154	LEU	N-CA-C	5.48	118.16	109.50
5	F	584	ARG	N-CA-C	5.45	116.06	108.00
3	D	154	LEU	N-CA-C	5.45	118.10	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	697	LYS	CA-C-N	-5.43	114.20	119.90
2	C	697	LYS	C-N-CA	-5.43	114.20	119.90
2	I	109	ALA	CA-C-N	5.42	125.84	119.99
2	I	109	ALA	C-N-CA	5.42	125.84	119.99
1	G	192	VAL	N-CA-C	-5.42	102.07	109.55
3	J	48	THR	N-CA-C	-5.41	101.63	109.59
2	C	1316	GLU	CA-C-N	5.40	124.58	118.97
2	C	1316	GLU	C-N-CA	5.40	124.58	118.97
2	C	1160	ASP	N-CA-C	5.39	122.28	110.80
3	D	470	VAL	CA-C-N	5.37	126.55	119.84
3	D	470	VAL	C-N-CA	5.37	126.55	119.84
2	I	1106	ARG	N-CA-C	-5.33	101.75	109.59
1	G	29	GLU	N-CA-C	5.31	119.39	112.17
2	I	1160	ASP	N-CA-C	5.31	122.11	110.80
1	H	20	SER	CB-CA-C	-5.31	110.47	116.63
5	L	584	ARG	N-CA-C	5.31	115.86	108.00
2	I	1316	GLU	CA-C-N	5.28	124.46	118.97
2	I	1316	GLU	C-N-CA	5.28	124.46	118.97
3	D	450	HIS	CA-C-N	5.25	125.31	119.32
3	D	450	HIS	C-N-CA	5.25	125.31	119.32
3	J	450	HIS	CA-C-N	5.25	125.30	119.32
3	J	450	HIS	C-N-CA	5.25	125.30	119.32
4	E	15	ASN	N-CA-C	5.24	117.00	111.28
2	C	1106	ARG	N-CA-C	-5.24	101.23	109.25
1	A	29	GLU	N-CA-C	5.23	119.28	112.17
3	J	338	PHE	CA-C-N	-5.23	115.78	122.79
3	J	338	PHE	C-N-CA	-5.23	115.78	122.79
3	J	470	VAL	CA-C-N	5.21	126.36	119.84
3	J	470	VAL	C-N-CA	5.21	126.36	119.84
5	L	584	ARG	CB-CA-C	-5.19	109.08	116.34
3	J	63	GLY	CA-C-N	5.15	125.16	119.90
3	J	63	GLY	C-N-CA	5.15	125.16	119.90
3	D	419	HIS	CA-C-N	5.15	125.43	119.92
3	D	419	HIS	C-N-CA	5.15	125.43	119.92
3	J	419	HIS	CA-C-N	5.13	125.41	119.92
3	J	419	HIS	C-N-CA	5.13	125.41	119.92
2	I	1152	GLY	N-CA-C	5.09	121.84	114.67
3	D	63	GLY	CA-C-N	5.08	125.08	119.90
3	D	63	GLY	C-N-CA	5.08	125.08	119.90
3	J	246	PRO	CA-C-N	5.03	124.63	119.05
3	J	246	PRO	C-N-CA	5.03	124.63	119.05
3	J	1344	LEU	CB-CA-C	-5.02	110.40	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	584	ARG	CB-CA-C	-5.02	109.31	116.34

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
5	L	601	PRO	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	1730	0	1756	50	0
1	B	1687	0	1700	53	0
1	G	1750	0	1764	45	0
1	H	1667	0	1689	53	0
2	C	10570	0	10582	263	0
2	I	10566	0	10576	245	0
3	D	9107	0	9308	248	0
3	J	9638	0	9853	262	0
4	E	691	0	695	14	0
4	K	627	0	634	10	0
5	F	3822	0	3885	91	0
5	L	3821	0	3884	98	0
6	C	20	0	11	2	0
6	I	20	0	11	2	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	55722	0	56348	1312	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 12.

All (1312) 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)
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.54	0.90
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.54	0.90
3:D:418:GLU:HG3	4:E:45:LYS:H	1.41	0.85
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.42	0.84
3:J:418:GLU:HG3	4:K:45:LYS:H	1.44	0.81
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.61	0.81
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.45	0.81
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.62	0.81
2:I:452:ARG:NH1	2:I:584:TYR:O	2.14	0.81
3:J:1171:GLY:HA2	3:J:1193:TRP:HZ3	1.45	0.81
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.63	0.80
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.46	0.80
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.63	0.80
3:J:342:LEU:HD11	3:J:1324:SER:HB3	1.64	0.80
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.62	0.79
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.64	0.79
2:C:452:ARG:NH1	2:C:584:TYR:O	2.15	0.79
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.64	0.79
3:D:1171:GLY:HA2	3:D:1193:TRP:HZ3	1.45	0.78
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.64	0.78
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.65	0.78
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.65	0.77
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.65	0.77
2:C:1248:THR:HG21	5:F:531:PRO:HG3	1.67	0.76
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.18	0.76
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.69	0.75
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.68	0.75
2:C:18:ARG:NH1	2:C:621:SER:O	2.20	0.75
2:I:18:ARG:NH1	2:I:621:SER:O	2.19	0.74
5:L:97:PRO:HA	5:L:100:MET:HG3	1.69	0.74
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.71	0.73
5:F:97:PRO:HA	5:F:100:MET:HG3	1.70	0.73
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.71	0.72
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.55	0.72
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.72	0.71
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.74	0.70
1:G:226:GLU:HG2	1:H:10:LYS:HE3	1.74	0.70
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.55	0.70
1:G:45:ARG:NH1	1:H:34:GLY:O	2.25	0.70
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.75	0.69
1:G:10:LYS:HE2	1:H:229:GLU:HB3	1.75	0.69
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.59	0.68
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.58	0.68
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.58	0.68
3:D:1297:LYS:HG2	3:J:1302:TYR:O	1.92	0.68
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.75	0.68
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.76	0.68
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.75	0.68
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.76	0.68
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.76	0.68
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.75	0.67
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.59	0.67
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.76	0.67
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.76	0.67
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.77	0.67
3:J:576:ARG:NH1	3:J:593:ASN:O	2.28	0.67
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.75	0.67
3:D:576:ARG:NH1	3:D:593:ASN:O	2.28	0.67
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.75	0.67
1:A:224:LEU:HD22	1:B:228:LEU:HD11	1.76	0.67
1:B:90:VAL:HG11	1:B:146:VAL:HG11	1.77	0.67
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.77	0.67
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.60	0.67
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.75	0.66
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.59	0.66
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.77	0.66
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.76	0.66
3:D:334:LYS:HG3	3:D:335:GLN:H	1.60	0.66
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.77	0.66
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.78	0.66
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.78	0.66
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.78	0.66
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:963:VAL:HB	3:J:980:THR:HG23	1.77	0.66
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.78	0.66
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.77	0.65
1:H:59:VAL:O	1:H:171:LEU:N	2.29	0.65
3:J:1206:ARG:NH2	3:J:1223:LEU:O	2.28	0.65
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.29	0.65
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.78	0.65
1:A:166:ARG:O	1:A:168:ILE:N	2.30	0.65
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.79	0.65
2:I:452:ARG:NH2	2:I:458:GLU:OE2	2.29	0.65
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	1.78	0.65
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.78	0.65
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.30	0.64
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.30	0.64
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.79	0.64
5:L:316:PHE:HZ	5:L:334:SER:HA	1.63	0.64
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.64
1:H:90:VAL:HG11	1:H:146:VAL:HG11	1.80	0.64
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.77	0.64
3:J:79:LYS:HB2	5:L:569:THR:H	1.63	0.64
2:C:120:GLN:HG3	2:C:121:GLU:HG3	1.80	0.64
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.80	0.64
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.80	0.64
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.79	0.63
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.79	0.63
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.78	0.63
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.79	0.63
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.80	0.63
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.81	0.63
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.79	0.63
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.64	0.63
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.81	0.63
5:F:316:PHE:HZ	5:F:334:SER:HA	1.63	0.63
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.32	0.63
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.81	0.63
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.81	0.62
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.81	0.62
5:F:134:VAL:HA	5:F:273:MET:HE1	1.81	0.62
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.82	0.62
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.82	0.62
1:A:12:ARG:HG3	1:B:230:ALA:HB1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.64	0.62
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.81	0.62
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.80	0.62
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.81	0.62
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.80	0.62
3:J:961:SER:HB2	3:J:981:GLU:HB3	1.81	0.62
5:L:134:VAL:HA	5:L:273:MET:HE1	1.82	0.62
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.32	0.62
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.81	0.62
2:C:109:ALA:HB1	2:C:110:PRO:C	2.24	0.62
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.82	0.62
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.33	0.62
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.81	0.62
2:I:745:GLU:HG3	2:I:1017:GLN:HB3	1.81	0.62
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.82	0.62
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.65	0.61
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.33	0.61
3:J:136:GLU:OE2	3:J:312:ARG:NH1	2.33	0.61
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.32	0.61
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.82	0.61
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.83	0.61
3:J:722:ILE:HA	3:J:725:MET:HE3	1.82	0.61
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.65	0.61
2:C:136:PHE:O	2:C:143:ARG:N	2.30	0.61
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.83	0.61
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.83	0.61
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.82	0.60
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.65	0.60
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.83	0.60
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.83	0.60
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.83	0.60
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.81	0.60
2:I:30:ILE:HD12	2:I:30:ILE:H	1.65	0.60
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.83	0.60
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.82	0.60
2:I:499:SER:O	2:I:503:LYS:HB2	2.02	0.60
3:J:128:LEU:HA	3:J:192:MET:HE1	1.84	0.60
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.84	0.60
3:D:722:ILE:HA	3:D:725:MET:HE3	1.82	0.60
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.66	0.60
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.83	0.59
3:D:128:LEU:HA	3:D:192:MET:HE1	1.83	0.59
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.85	0.59
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.83	0.59
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.30	0.59
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.84	0.59
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.83	0.59
2:C:1272:GLU:HB2	3:D:342:LEU:O	2.02	0.59
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.84	0.59
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.83	0.59
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.83	0.59
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.85	0.59
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.83	0.59
2:C:88:ARG:NE	2:C:1040:ASP:OD1	2.27	0.59
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.84	0.59
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.17	0.58
2:C:499:SER:O	2:C:503:LYS:HB2	2.03	0.58
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.85	0.58
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.35	0.58
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.86	0.58
3:D:650:LYS:NZ	3:D:765:GLU:OE2	2.35	0.58
2:I:705:GLU:HB2	2:I:794:LEU:H	1.68	0.58
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.39	0.58
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.86	0.58
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.84	0.58
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.86	0.58
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.86	0.58
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.84	0.58
2:C:705:GLU:HB2	2:C:794:LEU:H	1.68	0.58
2:I:930:ASP:OD2	2:I:931:VAL:N	2.37	0.58
3:D:334:LYS:CG	3:D:335:GLN:H	2.17	0.58
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.67	0.58
3:J:293:ARG:NH1	5:L:104:GLU:OE2	2.35	0.58
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.39	0.58
5:F:343:LYS:HD2	5:F:343:LYS:H	1.68	0.58
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.67	0.58
3:D:1171:GLY:HA2	3:D:1193:TRP:CZ3	2.34	0.58
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.69	0.58
1:B:95:LYS:HZ3	1:B:98:VAL:HG23	1.68	0.58
3:D:334:LYS:HG3	3:D:335:GLN:N	2.18	0.58
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:293:ARG:NH1	5:F:104:GLU:OE2	2.35	0.57
1:G:12:ARG:H	1:G:30:PRO:HD2	1.69	0.57
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.85	0.57
1:A:231:PHE:CZ	1:B:221:ALA:HB3	2.39	0.57
2:C:930:ASP:OD2	2:C:931:VAL:N	2.37	0.57
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.84	0.57
3:D:749:LYS:HD3	3:D:753:SER:HB2	1.86	0.57
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.86	0.57
1:H:82:LEU:HD22	1:H:173:VAL:HG22	1.86	0.57
1:H:101:THR:H	1:H:116:THR:HG22	1.69	0.57
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.86	0.57
2:C:148:GLN:NE2	2:C:535:PRO:O	2.33	0.57
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.85	0.57
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.86	0.57
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.84	0.57
1:B:82:LEU:HD22	1:B:173:VAL:HG22	1.87	0.57
2:C:703:GLY:N	2:C:705:GLU:OE2	2.36	0.57
1:G:23:HIS:HB2	1:G:205:MET:O	2.04	0.57
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.68	0.57
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.86	0.57
3:J:958:ILE:HG23	3:J:982:LEU:HD11	1.87	0.57
5:L:547:VAL:HG23	5:L:603:ARG:HH11	1.69	0.57
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.87	0.57
1:B:101:THR:H	1:B:116:THR:HG22	1.69	0.57
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.69	0.57
5:F:395:THR:OG1	5:F:396:ASN:N	2.38	0.57
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.85	0.57
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.87	0.57
5:L:395:THR:OG1	5:L:396:ASN:N	2.38	0.57
1:A:12:ARG:H	1:A:30:PRO:HD2	1.69	0.57
3:D:709:ARG:C	3:D:711:GLY:H	2.13	0.57
5:L:343:LYS:H	5:L:343:LYS:HD2	1.69	0.57
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.87	0.56
3:J:709:ARG:C	3:J:711:GLY:H	2.13	0.56
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.32	0.56
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.85	0.56
3:J:46:TYR:HE1	5:L:456:MET:HE2	1.69	0.56
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.69	0.56
2:C:30:ILE:HD12	2:C:30:ILE:H	1.69	0.56
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.88	0.56
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.86	0.56
1:G:181:GLU:HB3	1:G:206:GLU:HG3	1.87	0.56
3:J:42:GLU:CG	5:L:451:ARG:HE	2.18	0.56
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.88	0.56
3:D:218:THR:HA	3:D:221:ILE:HG22	1.88	0.56
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.69	0.56
2:I:324:LYS:O	2:I:327:GLN:NE2	2.38	0.56
2:I:560:PRO:O	3:J:780:ARG:NH2	2.39	0.56
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.36	0.56
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.86	0.56
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.86	0.56
2:C:324:LYS:O	2:C:327:GLN:NE2	2.38	0.56
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.86	0.56
3:D:557:LYS:HA	3:D:563:LEU:HA	1.88	0.56
3:J:557:LYS:HA	3:J:563:LEU:HA	1.88	0.56
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.87	0.56
3:J:749:LYS:HD3	3:J:753:SER:HB2	1.87	0.56
3:J:1216:ALA:HB1	3:J:1218:HIS:HD2	1.69	0.56
2:I:71:VAL:HG21	2:I:118:LYS:HE2	1.88	0.56
2:I:528:ARG:NH2	2:I:576:SER:O	2.38	0.56
2:C:495:ALA:HB3	5:F:471:LEU:HD13	1.88	0.56
2:C:685:MET:HA	2:C:688:GLN:HE21	1.71	0.56
2:C:980:VAL:O	2:C:984:VAL:HB	2.06	0.56
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.88	0.56
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.88	0.56
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.87	0.56
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.87	0.55
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.20	0.55
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.88	0.55
1:H:182:ARG:NH1	3:J:581:MET:SD	2.79	0.55
2:I:685:MET:HA	2:I:688:GLN:HE21	1.72	0.55
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.87	0.55
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.71	0.55
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.88	0.55
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.88	0.55
1:B:64:VAL:HG12	1:B:65:LEU:H	1.70	0.55
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.86	0.55
2:C:71:VAL:HG21	2:C:118:LYS:HE2	1.87	0.55
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.89	0.55
2:C:808:ASN:H	3:D:633:ALA:HB2	1.72	0.55
3:D:642:ASP:HA	3:D:764:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.87	0.55
2:I:980:VAL:O	2:I:984:VAL:HB	2.06	0.55
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.88	0.55
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.89	0.55
2:I:109:ALA:HB1	2:I:110:PRO:C	2.31	0.55
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.89	0.55
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.88	0.55
3:J:218:THR:HA	3:J:221:ILE:HG22	1.88	0.55
2:C:528:ARG:NH2	2:C:576:SER:O	2.38	0.55
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.89	0.55
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.89	0.55
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.89	0.55
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.72	0.55
5:L:127:ILE:O	5:L:130:VAL:HG22	2.06	0.55
2:I:148:GLN:NE2	2:I:535:PRO:O	2.32	0.55
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.71	0.55
1:H:64:VAL:HG12	1:H:65:LEU:H	1.71	0.55
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.88	0.55
2:I:1272:GLU:HB2	3:J:342:LEU:O	2.07	0.55
1:A:23:HIS:HB2	1:A:205:MET:O	2.05	0.54
2:C:68:LEU:HD11	2:C:100:LEU:HB3	1.89	0.54
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.89	0.54
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.72	0.54
3:J:682:VAL:O	3:J:685:ILE:HG12	2.07	0.54
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.88	0.54
3:J:700:ASN:O	3:J:704:GLU:HB2	2.07	0.54
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.88	0.54
3:D:1227:HIS:HD2	3:J:1293:GLU:H	1.55	0.54
2:I:808:ASN:H	3:J:633:ALA:HB2	1.73	0.54
5:L:315:TRP:HZ2	5:L:341:LEU:HD21	1.72	0.54
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.89	0.54
5:F:315:TRP:HZ2	5:F:341:LEU:HD21	1.72	0.54
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.89	0.54
1:A:14:VAL:HG22	1:A:15:ASP:H	1.72	0.54
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.89	0.54
2:C:560:PRO:O	3:D:780:ARG:NH2	2.40	0.54
3:D:394:ILE:HG23	5:F:536:THR:HG22	1.89	0.54
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.72	0.54
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.88	0.54
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.88	0.54
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.88	0.54
2:I:778:GLU:O	2:I:781:ASP:HB2	2.07	0.54
3:J:654:ILE:O	3:J:658:GLU:HB2	2.08	0.54
2:I:878:THR:OG1	2:I:879:GLY:N	2.39	0.54
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.90	0.54
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.08	0.54
1:A:181:GLU:HB3	1:A:206:GLU:HG3	1.88	0.54
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.56	0.54
4:E:10:VAL:HG13	4:E:16:ARG:HB2	1.90	0.54
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.22	0.54
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.89	0.54
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.90	0.54
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.71	0.54
2:I:68:LEU:HD11	2:I:100:LEU:HB3	1.89	0.54
3:J:514:THR:HB	3:J:576:ARG:HG2	1.90	0.54
3:J:901:ARG:HA	3:J:908:ILE:HA	1.89	0.54
2:C:778:GLU:O	2:C:781:ASP:HB2	2.08	0.53
3:D:700:ASN:O	3:D:704:GLU:HB2	2.08	0.53
3:D:1290:ARG:HG2	3:D:1298:VAL:HG12	1.89	0.53
1:H:95:LYS:NZ	1:H:98:VAL:HG23	2.23	0.53
2:C:878:THR:OG1	2:C:879:GLY:N	2.38	0.53
3:D:1216:ALA:HB1	3:D:1218:HIS:HD2	1.73	0.53
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.73	0.53
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.41	0.53
2:I:703:GLY:N	2:I:705:GLU:OE2	2.38	0.53
3:J:1290:ARG:HG2	3:J:1298:VAL:HG12	1.89	0.53
3:D:682:VAL:O	3:D:685:ILE:HG12	2.08	0.53
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.90	0.53
3:D:514:THR:HB	3:D:576:ARG:HG2	1.90	0.53
3:D:901:ARG:HA	3:D:908:ILE:HA	1.90	0.53
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.42	0.53
5:L:94:THR:OG1	5:L:95:THR:N	2.41	0.53
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.91	0.53
3:D:654:ILE:O	3:D:658:GLU:HB2	2.08	0.53
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.08	0.53
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.90	0.53
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.91	0.53
1:B:101:THR:HG22	1:B:116:THR:HB	1.91	0.53
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.90	0.53
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.90	0.53
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.90	0.53
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.91	0.53
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.73	0.53
3:J:210:SER:O	3:J:214:ARG:HG2	2.08	0.53
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.73	0.52
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.90	0.52
5:L:479:THR:HG23	5:L:481:GLU:H	1.74	0.52
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.74	0.52
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.74	0.52
3:D:111:THR:O	3:D:239:LEU:N	2.39	0.52
3:D:210:SER:O	3:D:214:ARG:HG2	2.09	0.52
3:D:251:PRO:HD2	5:F:507:MET:HE1	1.90	0.52
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.91	0.52
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.91	0.52
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.92	0.52
3:J:335:GLN:HG2	3:J:343:LEU:HD11	1.92	0.52
3:J:847:ASP:OD1	3:J:847:ASP:N	2.31	0.52
3:J:1171:GLY:HA2	3:J:1193:TRP:CZ3	2.35	0.52
5:F:573:LEU:H	5:F:573:LEU:HD23	1.73	0.52
3:J:514:THR:OG1	3:J:594:GLN:O	2.26	0.52
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.91	0.52
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.10	0.52
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.92	0.52
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.74	0.52
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.90	0.52
3:J:527:LEU:HD21	3:J:536:LEU:HG	1.92	0.52
3:D:1372:ARG:HH21	3:J:854:ALA:HB3	1.75	0.52
1:G:14:VAL:HG22	1:G:15:ASP:H	1.74	0.52
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.91	0.52
3:J:825:VAL:C	3:J:826:ILE:HG13	2.35	0.52
2:C:316:GLU:CD	2:C:316:GLU:H	2.18	0.52
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	1.92	0.52
5:F:479:THR:HG23	5:F:481:GLU:H	1.74	0.52
2:I:30:ILE:HD11	2:I:575:LEU:HD22	1.91	0.52
2:I:316:GLU:H	2:I:316:GLU:CD	2.18	0.52
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.91	0.52
2:C:90:VAL:HG12	2:C:91:THR:H	1.75	0.52
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	1.91	0.52
5:L:166:VAL:O	5:L:167:ASP:HB2	2.10	0.52
2:C:125:GLY:HA2	2:C:499:SER:HB2	1.91	0.52
5:F:166:VAL:O	5:F:167:ASP:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:594:VAL:HG22	2:I:599:VAL:HA	1.92	0.52
3:J:1266:ILE:HA	3:J:1302:TYR:HA	1.92	0.52
5:L:573:LEU:HD23	5:L:573:LEU:H	1.75	0.52
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.92	0.52
5:F:246:GLN:HE21	5:F:249:ILE:HD12	1.75	0.52
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.92	0.52
3:J:843:VAL:HG11	3:J:897:HIS:O	2.10	0.52
2:C:250:THR:HA	2:C:268:ARG:HA	1.92	0.51
2:I:250:THR:HA	2:I:268:ARG:HA	1.92	0.51
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.92	0.51
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.92	0.51
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.92	0.51
2:C:109:ALA:HB1	2:C:111:GLU:HA	1.91	0.51
1:G:41:ASN:ND2	2:I:1216:ARG:O	2.43	0.51
1:H:101:THR:HG22	1:H:116:THR:HB	1.91	0.51
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.91	0.51
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.76	0.51
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.91	0.51
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.32	0.51
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.93	0.51
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.92	0.51
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.75	0.51
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.45	0.51
3:D:1155:ILE:HD12	3:D:1210:ILE:HB	1.91	0.51
2:I:206:ALA:O	2:I:209:ILE:HG22	2.11	0.51
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	1.90	0.51
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.92	0.51
3:D:514:THR:OG1	3:D:594:GLN:O	2.27	0.51
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.11	0.51
2:I:1223:ARG:NH1	3:J:721:SER:OG	2.34	0.51
3:J:1155:ILE:HD12	3:J:1210:ILE:HB	1.91	0.51
2:C:555:TYR:HD2	6:C:1401:42S:H1	1.76	0.51
5:F:486:ARG:HB2	5:F:486:ARG:CZ	2.41	0.51
2:I:555:TYR:HD2	6:I:1401:42S:H1	1.76	0.51
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.92	0.51
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.75	0.51
5:F:483:LEU:HD12	5:F:483:LEU:H	1.75	0.51
5:L:246:GLN:HE21	5:L:249:ILE:HD12	1.75	0.51
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.11	0.51
2:C:206:ALA:O	2:C:209:ILE:HG22	2.11	0.50
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:978:ARG:HB2	3:J:1199:PHE:CZ	2.45	0.50
5:L:314:THR:O	5:L:318:ALA:HB3	2.12	0.50
3:D:527:LEU:HD21	3:D:536:LEU:HG	1.93	0.50
2:I:4:SER:OG	2:I:5:TYR:N	2.42	0.50
2:I:109:ALA:HB1	2:I:111:GLU:HA	1.93	0.50
2:I:201:ARG:NH2	2:I:370:MET:O	2.38	0.50
3:D:825:VAL:C	3:D:826:ILE:HG13	2.35	0.50
5:L:164:GLY:O	5:L:260:ARG:HB2	2.11	0.50
1:B:6:THR:O	1:B:6:THR:OG1	2.24	0.50
2:C:400:VAL:HG11	2:C:452:ARG:HD2	1.93	0.50
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.93	0.50
1:G:90:VAL:HG23	1:G:123:ILE:HD13	1.94	0.50
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.93	0.50
2:I:13:LYS:NZ	2:I:1148:ALA:O	2.45	0.50
3:J:1184:ASP:O	3:J:1186:TYR:N	2.45	0.50
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.93	0.50
2:C:618:GLN:HG3	2:C:620:ASN:H	1.77	0.50
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.76	0.50
2:I:90:VAL:HG12	2:I:91:THR:H	1.77	0.50
2:I:115:LYS:HE3	2:I:116:ASP:H	1.77	0.50
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.94	0.50
3:J:973:LEU:HD23	3:J:1003:LEU:HD12	1.94	0.50
2:C:4:SER:OG	2:C:5:TYR:N	2.41	0.50
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.92	0.50
2:I:618:GLN:HG3	2:I:620:ASN:H	1.76	0.50
1:A:172:LEU:HD12	1:A:172:LEU:H	1.76	0.50
1:A:231:PHE:CE1	1:B:221:ALA:HB3	2.47	0.50
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.47	0.50
2:C:594:VAL:HG22	2:C:599:VAL:HA	1.93	0.50
3:D:843:VAL:HG11	3:D:897:HIS:O	2.11	0.50
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.77	0.50
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.77	0.50
3:D:152:THR:OG1	3:D:153:ASN:N	2.44	0.50
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.12	0.50
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.75	0.49
2:C:642:SER:HB2	3:D:770:LEU:HD21	1.93	0.49
3:D:19:ALA:O	3:D:20:ILE:HG13	2.11	0.49
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.94	0.49
4:E:71:GLU:HA	4:E:74:GLU:HG3	1.94	0.49
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.27	0.49
2:C:871:VAL:O	2:C:944:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.93	0.49
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.92	0.49
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.93	0.49
1:A:45:ARG:HG2	1:B:38:THR:HB	1.94	0.49
1:A:90:VAL:HG23	1:A:123:ILE:HD13	1.94	0.49
2:C:870:ILE:HG21	2:C:931:VAL:HG11	1.94	0.49
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.45	0.49
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.77	0.49
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.27	0.49
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.47	0.49
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.45	0.49
5:F:164:GLY:O	5:F:260:ARG:HB2	2.12	0.49
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.94	0.49
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.94	0.49
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.95	0.49
1:G:172:LEU:HD12	1:G:172:LEU:H	1.77	0.49
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.94	0.49
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.45	0.49
3:J:19:ALA:O	3:J:20:ILE:HG13	2.12	0.49
3:J:827:GLU:C	3:J:829:GLY:H	2.19	0.49
2:C:13:LYS:NZ	2:C:1148:ALA:O	2.46	0.49
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.94	0.49
5:L:486:ARG:HB2	5:L:486:ARG:CZ	2.43	0.49
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.94	0.49
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.94	0.49
4:E:38:LEU:HD23	4:E:58:LEU:HD13	1.93	0.49
5:F:314:THR:O	5:F:318:ALA:HB3	2.12	0.49
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.45	0.49
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.47	0.49
2:C:30:ILE:HD11	2:C:575:LEU:HD22	1.93	0.49
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.28	0.49
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.95	0.49
5:L:561:MET:HA	5:L:567:MET:HE1	1.94	0.49
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.95	0.49
2:I:642:SER:HB2	3:J:770:LEU:HD21	1.95	0.49
2:I:829:THR:HA	2:I:1059:ARG:HA	1.95	0.49
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.95	0.49
3:J:849:LEU:HB3	3:J:853:THR:HG23	1.95	0.49
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.95	0.49
5:F:561:MET:HA	5:F:567:MET:HE1	1.95	0.49
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1366:HIS:O	3:J:1370:MET:N	2.39	0.49
2:C:201:ARG:NH2	2:C:370:MET:O	2.39	0.48
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.46	0.48
3:J:77:ARG:HB3	3:J:80:HIS:ND1	2.28	0.48
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.48	0.48
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.94	0.48
2:I:557:ARG:HH21	2:I:607:SER:C	2.21	0.48
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.95	0.48
2:I:896:THR:HB	2:I:897:PRO:HD2	1.95	0.48
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.79	0.48
2:C:115:LYS:HE3	2:C:116:ASP:H	1.77	0.48
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.96	0.48
1:H:95:LYS:HZ3	1:H:98:VAL:HG23	1.78	0.48
2:I:870:ILE:HG21	2:I:931:VAL:HG11	1.94	0.48
2:C:557:ARG:HH21	2:C:607:SER:C	2.21	0.48
3:D:356:THR:OG1	3:D:357:VAL:N	2.47	0.48
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.48	0.48
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.94	0.48
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.96	0.48
2:I:1065:LYS:HE2	3:J:462:ASP:O	2.14	0.48
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.13	0.48
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.96	0.48
2:C:478:ARG:HG2	2:C:492:MET:HG2	1.96	0.48
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.78	0.48
2:C:490:GLN:HG2	2:C:491:ASP:N	2.27	0.48
3:D:1184:ASP:O	3:D:1186:TYR:N	2.45	0.48
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.29	0.48
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.94	0.48
3:D:113:HIS:HD1	3:D:115:TRP:H	1.61	0.48
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.96	0.48
3:J:613:GLY:O	3:J:617:THR:OG1	2.29	0.48
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.14	0.48
2:C:886:LYS:H	2:C:917:SER:HB3	1.79	0.48
2:C:896:THR:HB	2:C:897:PRO:HD2	1.94	0.48
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.95	0.48
2:I:593:LYS:HE3	2:I:595:THR:HG22	1.96	0.48
2:I:886:LYS:H	2:I:917:SER:HB3	1.79	0.48
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.96	0.48
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.95	0.48
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.96	0.48
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:23:ASP:OD1	2:C:23:ASP:N	2.46	0.48
2:I:478:ARG:HG2	2:I:492:MET:HG2	1.96	0.48
3:J:111:THR:O	3:J:239:LEU:N	2.40	0.48
5:L:483:LEU:HD12	5:L:483:LEU:H	1.79	0.48
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.96	0.48
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.29	0.48
3:D:77:ARG:HB3	3:D:80:HIS:ND1	2.28	0.48
3:D:600:ALA:O	3:D:603:LYS:HG2	2.14	0.48
1:H:218:ARG:O	1:H:222:THR:OG1	2.26	0.48
3:J:298:MET:SD	5:L:402:LEU:HB3	2.53	0.48
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.95	0.48
1:H:134:THR:HG23	1:H:135:ASP:N	2.29	0.48
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.13	0.48
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.79	0.48
2:I:582:ASN:HB3	2:I:586:PHE:H	1.78	0.48
5:L:602:SER:OG	5:L:603:ARG:N	2.47	0.48
2:C:724:VAL:HG23	2:C:775:GLU:O	2.14	0.47
2:C:980:VAL:HA	2:C:984:VAL:HA	1.96	0.47
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.41	0.47
3:D:800:LEU:O	3:D:803:VAL:HG12	2.14	0.47
3:D:810:THR:HG23	3:D:811:GLU:H	1.78	0.47
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.96	0.47
3:J:645:VAL:HB	3:J:701:LEU:HD23	1.96	0.47
3:J:694:SER:OG	3:J:738:ARG:NE	2.47	0.47
3:J:698:MET:O	3:J:702:GLN:HB3	2.14	0.47
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.95	0.47
2:C:1065:LYS:HE2	3:D:462:ASP:O	2.15	0.47
2:C:1184:THR:HG23	2:C:1189:GLY:HA3	1.96	0.47
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.95	0.47
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.95	0.47
2:C:692:THR:OG1	2:C:693:LEU:N	2.45	0.47
2:C:829:THR:HA	2:C:1059:ARG:HA	1.95	0.47
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.96	0.47
1:G:83:LEU:HD23	2:I:694:ARG:NH2	2.30	0.47
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.97	0.47
3:D:694:SER:OG	3:D:738:ARG:NE	2.47	0.47
2:I:1184:THR:HG23	2:I:1189:GLY:HA3	1.97	0.47
3:J:800:LEU:O	3:J:803:VAL:HG12	2.15	0.47
3:J:901:ARG:HD2	3:J:906:GLY:O	2.14	0.47
3:D:698:MET:O	3:D:702:GLN:HB3	2.14	0.47
3:D:849:LEU:HB3	3:D:853:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1347:LEU:HG	3:D:1357:ILE:HG23	1.97	0.47
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.45	0.47
2:I:496:LYS:HE3	2:I:496:LYS:HB3	1.65	0.47
3:J:113:HIS:HD1	3:J:115:TRP:H	1.63	0.47
3:J:152:THR:OG1	3:J:153:ASN:N	2.44	0.47
3:J:290:ILE:H	3:J:290:ILE:HD12	1.79	0.47
3:J:1347:LEU:HG	3:J:1357:ILE:HG23	1.97	0.47
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.96	0.47
3:D:298:MET:SD	5:F:402:LEU:HB3	2.54	0.47
3:D:708:ASN:OD1	3:D:708:ASN:N	2.48	0.47
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.96	0.47
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.97	0.47
2:C:470:ARG:NE	2:C:497:PRO:HB3	2.30	0.47
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.96	0.47
3:D:857:LEU:HD12	3:D:858:VAL:H	1.79	0.47
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.47	0.47
5:F:580:PHE:C	5:F:582:VAL:H	2.23	0.47
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.97	0.47
2:I:724:VAL:HG23	2:I:775:GLU:O	2.15	0.47
2:I:980:VAL:HA	2:I:984:VAL:HA	1.96	0.47
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.15	0.47
5:L:244:THR:O	5:L:247:GLU:HG2	2.15	0.47
1:A:22:THR:HB	1:A:206:GLU:OE2	2.15	0.47
3:D:901:ARG:HD2	3:D:906:GLY:O	2.15	0.47
4:E:50:ALA:O	4:E:54:ILE:HG12	2.15	0.47
1:B:134:THR:HG23	1:B:135:ASP:N	2.29	0.47
3:D:1366:HIS:O	3:D:1370:MET:N	2.40	0.47
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.50	0.47
2:I:811:ASN:C	2:I:815:SER:HB2	2.40	0.47
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.96	0.47
2:C:593:LYS:HE3	2:C:595:THR:HG22	1.97	0.47
2:C:811:ASN:C	2:C:815:SER:HB2	2.40	0.47
2:C:1247:SER:HB3	3:D:375:GLU:O	2.15	0.47
2:C:1262:LYS:HB2	2:C:1264:GLN:HB3	1.97	0.47
2:C:1271:GLY:HA2	3:D:344:GLY:HA2	1.97	0.47
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.15	0.47
5:F:602:SER:OG	5:F:603:ARG:N	2.47	0.47
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.96	0.47
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.97	0.47
2:I:494:ASN:HD22	2:I:497:PRO:HD3	1.80	0.47
2:I:692:THR:OG1	2:I:693:LEU:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.15	0.47
3:J:810:THR:HG23	3:J:811:GLU:H	1.79	0.47
1:B:218:ARG:O	1:B:222:THR:OG1	2.26	0.46
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.45	0.46
2:C:170:VAL:HG23	2:C:171:LEU:N	2.30	0.46
5:F:98:VAL:HB	5:F:402:LEU:HD11	1.96	0.46
5:F:499:LYS:HB2	5:F:499:LYS:HE3	1.76	0.46
2:I:1161:LEU:HD12	2:I:1161:LEU:HA	1.56	0.46
3:D:807:LEU:HD23	3:D:915:ILE:HG13	1.96	0.46
2:I:170:VAL:HG23	2:I:171:LEU:N	2.30	0.46
2:I:470:ARG:NE	2:I:497:PRO:HB3	2.31	0.46
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.81	0.46
2:I:1271:GLY:HA2	3:J:344:GLY:HA2	1.97	0.46
5:L:130:VAL:HB	5:L:365:MET:HG3	1.95	0.46
5:L:292:VAL:HG21	5:L:299:LYS:HG2	1.98	0.46
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.79	0.46
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.56	0.46
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.96	0.46
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.96	0.46
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.97	0.46
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.80	0.46
3:D:645:VAL:HB	3:D:701:LEU:HD23	1.96	0.46
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.96	0.46
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.97	0.46
3:J:42:GLU:OE1	3:J:42:GLU:N	2.49	0.46
2:C:42:ASP:OD2	2:C:46:GLN:HB3	2.15	0.46
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.47	0.46
3:D:56:LEU:HD12	3:D:56:LEU:H	1.80	0.46
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.97	0.46
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.48	0.46
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.98	0.46
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.51	0.46
1:A:195:ARG:HG2	1:A:198:LEU:HG	1.96	0.46
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.50	0.46
3:D:709:ARG:O	3:D:711:GLY:N	2.45	0.46
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.51	0.46
3:J:56:LEU:HD12	3:J:56:LEU:H	1.80	0.46
3:J:527:LEU:HD22	3:J:533:ALA:HA	1.97	0.46
3:J:600:ALA:O	3:J:603:LYS:HG2	2.15	0.46
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.55	0.46
2:C:494:ASN:HD22	2:C:497:PRO:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.97	0.46
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.16	0.46
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.49	0.46
1:H:149:GLY:HA3	1:H:177:TYR:CD2	2.50	0.46
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.97	0.46
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.98	0.46
3:D:746:LEU:HD23	3:D:758:PRO:HG3	1.98	0.46
5:F:281:ARG:O	5:F:285:ARG:HG3	2.15	0.46
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.97	0.46
5:F:569:THR:OG1	5:F:570:ASP:N	2.49	0.46
1:G:22:THR:HB	1:G:206:GLU:OE2	2.15	0.46
2:I:1101:LEU:HD23	3:J:725:MET:SD	2.56	0.46
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.47	0.46
2:I:1247:SER:HB3	3:J:375:GLU:O	2.16	0.46
3:J:436:ALA:HB3	3:J:485:MET:HA	1.97	0.46
3:J:857:LEU:HD12	3:J:858:VAL:H	1.80	0.46
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.96	0.46
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.98	0.46
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.78	0.46
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.97	0.46
5:L:569:THR:OG1	5:L:570:ASP:N	2.48	0.46
3:D:77:ARG:HG3	3:D:79:LYS:H	1.81	0.46
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.15	0.46
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.98	0.46
2:I:301:TYR:HB2	2:I:311:CYS:SG	2.56	0.46
2:I:498:ILE:HD12	2:I:498:ILE:H	1.81	0.46
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.96	0.46
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.48	0.46
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.98	0.46
5:L:580:PHE:C	5:L:582:VAL:H	2.22	0.46
2:C:24:VAL:HG21	2:C:704:MET:SD	2.57	0.46
2:C:548:ARG:HB3	2:C:569:ILE:O	2.16	0.46
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.97	0.46
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.98	0.46
2:I:548:ARG:HB3	2:I:569:ILE:O	2.15	0.46
3:J:746:LEU:HD23	3:J:758:PRO:HG3	1.98	0.46
3:D:361:LEU:HD22	3:D:365:GLN:HG3	1.98	0.45
5:F:244:THR:O	5:F:247:GLU:HG2	2.16	0.45
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.98	0.45
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.97	0.45
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ALA:HB2	1:B:128:HIS:HB3	1.99	0.45
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.98	0.45
3:D:42:GLU:OE1	3:D:42:GLU:N	2.49	0.45
3:D:395:LYS:HG2	5:F:536:THR:HG21	1.97	0.45
3:D:436:ALA:HB3	3:D:485:MET:HA	1.98	0.45
3:D:470:VAL:HA	3:D:471:PRO:HD3	1.76	0.45
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.44	0.45
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.25	0.45
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.51	0.45
5:F:532:LEU:HD12	5:F:532:LEU:H	1.82	0.45
3:J:416:ILE:HG12	3:J:441:LEU:HD21	1.99	0.45
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.98	0.45
1:A:13:LEU:HD23	1:A:13:LEU:H	1.81	0.45
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.79	0.45
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.97	0.45
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.50	0.45
3:J:950:ILE:HG13	3:J:1020:TRP:HZ3	1.81	0.45
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.51	0.45
2:C:149:LEU:HB2	2:C:530:ILE:CG2	2.47	0.45
3:D:290:ILE:HD12	3:D:290:ILE:H	1.81	0.45
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.51	0.45
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.99	0.45
3:J:317:THR:HB	3:J:324:LEU:HB3	1.98	0.45
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.97	0.45
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.99	0.45
2:C:490:GLN:HG3	5:F:472:GLN:OE1	2.17	0.45
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.70	0.45
3:D:527:LEU:HD22	3:D:533:ALA:HA	1.98	0.45
3:D:847:ASP:OD1	3:D:847:ASP:N	2.30	0.45
1:H:35:PHE:HA	1:H:38:THR:HG22	1.99	0.45
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.97	0.45
4:K:36:ASP:HB2	4:K:37:PRO:HD2	1.99	0.45
3:D:793:SER:O	3:D:797:THR:HG23	2.17	0.45
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.99	0.45
2:I:56:VAL:HG11	2:I:468:LEU:HB3	1.99	0.45
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.68	0.45
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.80	0.45
3:J:858:VAL:HA	3:J:859:PRO:HD3	1.77	0.45
3:J:984:LEU:HB2	3:J:993:GLU:HB2	1.99	0.45
2:C:245:ARG:HG2	2:C:337:PHE:CZ	2.52	0.45
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:24:VAL:HG21	2:I:704:MET:SD	2.56	0.45
2:I:1262:LYS:HB2	2:I:1264:GLN:HB3	1.97	0.45
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.98	0.45
5:L:499:LYS:HB2	5:L:499:LYS:HE3	1.77	0.45
5:F:292:VAL:HG21	5:F:299:LYS:HG2	1.98	0.45
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.98	0.45
3:J:620:PHE:O	3:J:624:ILE:HG13	2.16	0.45
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.50	0.45
4:K:38:LEU:HD23	4:K:58:LEU:HD13	1.99	0.45
1:A:145:LYS:HB3	1:A:145:LYS:HE3	1.79	0.45
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.88	0.45
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.51	0.45
1:B:196:THR:HG23	3:D:443:GLU:HG3	1.99	0.45
2:C:3:TYR:HE1	2:C:11:ILE:HD11	1.81	0.45
2:C:582:ASN:HB3	2:C:586:PHE:H	1.82	0.45
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.56	0.45
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.52	0.45
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.52	0.45
1:H:37:HIS:CE1	2:I:1216:ARG:HD2	2.52	0.45
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.99	0.45
2:I:3:TYR:HE1	2:I:11:ILE:HD11	1.82	0.45
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.49	0.45
2:I:515:MET:HE3	2:I:517:GLN:HB2	1.99	0.45
1:A:75:GLN:HA	2:C:729:ALA:N	2.32	0.45
1:B:151:GLY:O	1:B:177:TYR:HD2	2.00	0.45
2:C:40:GLU:O	2:C:73:TYR:OH	2.34	0.45
2:C:53:PHE:O	2:C:57:PHE:HB2	2.17	0.45
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.99	0.45
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.50	0.45
5:F:299:LYS:O	5:F:303:ILE:HG12	2.17	0.45
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.99	0.45
2:I:37:LYS:HA	2:I:37:LYS:HD3	1.78	0.45
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.52	0.45
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.52	0.45
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.98	0.45
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.81	0.44
2:C:1223:ARG:NH1	3:D:721:SER:OG	2.35	0.44
3:D:827:GLU:C	3:D:829:GLY:H	2.20	0.44
3:D:1149:ARG:CZ	3:D:1153:PRO:HG2	2.47	0.44
5:F:94:THR:HG23	5:F:96:ASP:OD1	2.17	0.44
1:H:33:ARG:NH1	2:I:1081:PRO:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:960:LEU:HB3	2:I:1025:PHE:CE2	2.52	0.44
3:J:733:SER:O	3:J:737:ILE:HG12	2.17	0.44
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.79	0.44
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.98	0.44
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.52	0.44
3:D:317:THR:HB	3:D:324:LEU:HB3	1.98	0.44
3:D:665:GLN:HG3	3:D:669:GLN:HE21	1.82	0.44
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.82	0.44
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.47	0.44
3:J:959:LYS:HB3	3:J:983:LYS:HB2	1.98	0.44
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.44
5:L:281:ARG:O	5:L:285:ARG:HG3	2.16	0.44
2:C:1160:ASP:HB2	2:C:1163:THR:OG1	2.17	0.44
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.97	0.44
3:D:418:GLU:O	3:D:420:PRO:HD3	2.17	0.44
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.53	0.44
2:I:1160:ASP:HB2	2:I:1163:THR:OG1	2.18	0.44
2:I:1341:ASP:HB3	2:I:1342:GLU:H	1.52	0.44
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.99	0.44
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.42	0.44
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.67	0.44
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.99	0.44
2:C:157:PHE:CZ	2:C:431:LYS:HG2	2.52	0.44
2:C:498:ILE:HD12	2:C:498:ILE:H	1.82	0.44
2:C:515:MET:HE3	2:C:517:GLN:HB2	1.98	0.44
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.81	0.44
3:D:1292:LEU:HD23	3:J:1226:VAL:HG11	1.98	0.44
5:F:130:VAL:HB	5:F:365:MET:HG3	1.98	0.44
5:F:461:ASN:O	5:F:465:ARG:HG2	2.17	0.44
2:I:53:PHE:O	2:I:57:PHE:HB2	2.17	0.44
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.99	0.44
3:J:248:ASP:O	3:J:251:PRO:HG3	2.18	0.44
3:J:665:GLN:HG3	3:J:669:GLN:HE21	1.82	0.44
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.99	0.44
1:A:44:ARG:HA	1:A:183:ILE:HG21	2.00	0.44
1:B:107:ILE:HG23	1:B:135:ASP:HA	2.00	0.44
2:C:69:GLN:HG3	2:C:101:ARG:HB3	1.99	0.44
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.67	0.44
3:D:248:ASP:O	3:D:251:PRO:HG3	2.18	0.44
3:D:279:LEU:HD11	3:D:296:LYS:HG2	2.00	0.44
1:H:41:ASN:O	1:H:45:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:40:GLU:O	2:I:73:TYR:OH	2.35	0.44
5:L:532:LEU:HD12	5:L:532:LEU:H	1.83	0.44
1:B:179:PRO:HA	1:B:208:ASN:ND2	2.32	0.44
1:G:47:LEU:O	1:G:180:VAL:HG21	2.17	0.44
1:H:112:ALA:HB2	1:H:128:HIS:HB3	1.99	0.44
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.52	0.44
2:I:490:GLN:HG2	2:I:491:ASP:N	2.31	0.44
3:J:708:ASN:OD1	3:J:708:ASN:N	2.50	0.44
3:J:709:ARG:O	3:J:711:GLY:N	2.45	0.44
3:J:1017:VAL:HG23	3:J:1018:ALA:H	1.81	0.44
5:L:461:ASN:O	5:L:465:ARG:HG2	2.18	0.44
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.99	0.44
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.99	0.44
2:I:1149:TYR:OH	2:I:1176:LEU:HD11	2.17	0.44
3:J:77:ARG:HG3	3:J:79:LYS:H	1.82	0.44
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.99	0.44
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.83	0.44
1:B:41:ASN:O	1:B:45:ARG:HG3	2.18	0.44
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.99	0.44
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.33	0.44
3:D:416:ILE:HG12	3:D:441:LEU:HD21	1.99	0.44
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.98	0.44
5:F:561:MET:HG2	5:F:576:VAL:HG22	2.00	0.44
3:J:548:VAL:HG12	3:J:550:VAL:HG13	2.00	0.44
3:J:827:GLU:O	3:J:829:GLY:N	2.37	0.44
5:L:299:LYS:O	5:L:303:ILE:HG12	2.18	0.44
5:F:99:ARG:HD3	5:F:99:ARG:HA	1.81	0.44
5:F:470:MET:HA	5:F:473:GLU:HB3	1.99	0.44
1:G:13:LEU:H	1:G:13:LEU:HD23	1.81	0.44
1:H:151:GLY:O	1:H:177:TYR:HD2	2.01	0.44
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.99	0.44
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.33	0.44
1:B:35:PHE:HA	1:B:38:THR:HG22	1.99	0.43
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.49	0.43
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.98	0.43
2:C:466:VAL:O	2:C:469:VAL:HG22	2.18	0.43
3:D:797:THR:O	3:D:801:VAL:HG13	2.18	0.43
3:D:806:ASP:O	3:D:808:VAL:HG23	2.18	0.43
3:D:1372:ARG:HH21	3:J:854:ALA:CB	2.31	0.43
5:F:281:ARG:HG2	5:F:285:ARG:HD2	2.00	0.43
1:G:207:THR:HG22	1:G:209:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.83	0.43
3:J:975:ILE:HD11	3:J:1003:LEU:HD11	2.00	0.43
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.53	0.43
2:C:117:ILE:HD12	2:C:488:MET:HG2	2.00	0.43
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.43
3:D:103:GLY:HA3	3:D:244:VAL:HG22	2.00	0.43
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.82	0.43
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.53	0.43
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.83	0.43
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.16	0.43
3:J:418:GLU:O	3:J:420:PRO:HD3	2.17	0.43
3:J:682:VAL:HA	3:J:685:ILE:HD13	2.00	0.43
5:L:470:MET:HA	5:L:473:GLU:HB3	1.99	0.43
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.34	0.43
2:C:27:LEU:HB2	2:C:524:ILE:HD11	2.00	0.43
2:C:738:GLU:HA	2:C:741:MET:HE2	2.00	0.43
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.17	0.43
3:D:860:ARG:HB3	3:D:861:ASN:H	1.54	0.43
3:D:888:CYS:SG	3:D:890:THR:HB	2.57	0.43
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	2.01	0.43
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.99	0.43
3:J:279:LEU:HD11	3:J:296:LYS:HG2	2.00	0.43
2:C:816:ILE:HG22	2:C:818:VAL:HG23	2.00	0.43
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.00	0.43
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.00	0.43
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.54	0.43
1:G:44:ARG:HA	1:G:183:ILE:HG21	2.00	0.43
3:J:46:TYR:CD1	5:L:452:ILE:HG22	2.53	0.43
5:L:571:TYR:HD1	5:L:575:GLU:HG2	1.82	0.43
1:A:74:VAL:HG22	1:A:76:GLU:H	1.83	0.43
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.99	0.43
2:C:179:TYR:OH	2:C:458:GLU:OE2	2.27	0.43
2:C:524:ILE:HG21	2:C:708:VAL:HG13	2.01	0.43
5:F:277:MET:HG3	5:F:362:ASN:ND2	2.33	0.43
5:F:513:ASP:C	5:F:515:GLU:H	2.26	0.43
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.33	0.43
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.33	0.43
2:I:524:ILE:HG21	2:I:708:VAL:HG13	2.01	0.43
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.54	0.43
5:L:281:ARG:HG2	5:L:285:ARG:HD2	2.01	0.43
1:A:47:LEU:O	1:A:180:VAL:HG21	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:83:GLN:O	2:C:87:ILE:HG13	2.19	0.43
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.53	0.43
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.01	0.43
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.84	0.43
3:D:123:ARG:HD2	3:D:1337:VAL:HG11	2.01	0.43
3:D:620:PHE:O	3:D:624:ILE:HG13	2.18	0.43
3:D:708:ASN:HB3	3:D:712:GLN:O	2.19	0.43
3:D:814:CYS:HB3	3:D:890:THR:OG1	2.18	0.43
2:I:239:MET:O	2:I:284:LEU:HD12	2.19	0.43
2:I:738:GLU:HA	2:I:741:MET:HE2	2.00	0.43
5:L:575:GLU:O	5:L:579:GLN:HG2	2.17	0.43
1:A:49:SER:OG	1:A:50:SER:N	2.51	0.43
1:B:67:GLU:O	1:B:78:ILE:HB	2.19	0.43
2:C:144:VAL:HG23	2:C:515:MET:HB2	2.00	0.43
2:C:960:LEU:HB3	2:C:1025:PHE:CE2	2.53	0.43
2:C:1149:TYR:OH	2:C:1176:LEU:HD11	2.18	0.43
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.00	0.43
5:F:245:ALA:O	5:F:249:ILE:HG13	2.17	0.43
1:G:74:VAL:HG22	1:G:76:GLU:H	1.84	0.43
2:I:27:LEU:HB2	2:I:524:ILE:HD11	1.99	0.43
2:I:55:SER:OG	2:I:56:VAL:N	2.52	0.43
2:I:69:GLN:HG3	2:I:101:ARG:HB3	2.00	0.43
2:I:1319:MET:HA	2:I:1320:PRO:HD3	1.94	0.43
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.18	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.59	0.43
2:C:1178:LYS:HA	2:C:1178:LYS:HD3	1.85	0.43
3:D:30:ILE:HG23	3:D:243:PRO:HG3	2.00	0.43
3:D:613:GLY:O	3:D:617:THR:OG1	2.29	0.43
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.51	0.43
5:F:476:ARG:HG3	5:F:477:GLU:N	2.33	0.43
2:I:168:GLY:C	2:I:170:VAL:H	2.27	0.43
2:I:976:ARG:HD2	2:I:989:LEU:HD23	2.00	0.43
2:I:1085:MET:HA	2:I:1085:MET:HE2	2.01	0.43
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	2.01	0.43
3:J:94:GLN:O	3:J:97:VAL:HG23	2.18	0.43
3:J:708:ASN:HB3	3:J:712:GLN:O	2.18	0.43
3:J:888:CYS:SG	3:J:890:THR:HB	2.58	0.43
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.84	0.43
5:L:280:VAL:HG22	5:L:347:ILE:HD13	2.00	0.43
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.44	0.43
2:C:1212:LEU:HD22	2:C:1225:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.84	0.43
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.99	0.43
2:I:1248:THR:HG21	5:L:531:PRO:HG3	2.01	0.43
2:I:1262:LYS:HA	2:I:1262:LYS:HD3	1.78	0.43
3:J:45:ASN:O	3:J:46:TYR:HD2	2.02	0.43
3:J:367:GLY:HA3	3:J:448:GLN:HB2	2.00	0.43
3:J:949:SER:HB3	3:J:1018:ALA:O	2.19	0.43
5:L:245:ALA:O	5:L:249:ILE:HG13	2.18	0.43
5:L:513:ASP:C	5:L:515:GLU:H	2.26	0.43
5:L:572:THR:O	5:L:576:VAL:HG23	2.18	0.43
3:D:141:PHE:HA	3:D:180:MET:HE2	2.00	0.43
3:D:515:ARG:HH21	3:D:717:VAL:HG23	1.84	0.43
3:D:733:SER:O	3:D:737:ILE:HG12	2.18	0.43
2:I:582:ASN:HB3	2:I:586:PHE:N	2.33	0.43
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.19	0.43
2:I:730:SER:O	2:I:753:LEU:HB2	2.19	0.43
3:J:103:GLY:HA3	3:J:244:VAL:HG22	2.01	0.43
3:J:141:PHE:HA	3:J:180:MET:HE2	2.00	0.43
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	2.01	0.43
5:L:296:LYS:HA	5:L:296:LYS:HD3	1.78	0.43
5:L:582:VAL:HG12	5:L:586:ARG:HG2	2.01	0.43
2:C:168:GLY:C	2:C:170:VAL:H	2.27	0.42
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.83	0.42
2:C:976:ARG:HD2	2:C:989:LEU:HD23	2.01	0.42
3:D:45:ASN:O	3:D:46:TYR:HD2	2.02	0.42
5:F:280:VAL:HG22	5:F:347:ILE:HD13	2.00	0.42
3:J:30:ILE:HG23	3:J:243:PRO:HG3	2.01	0.42
3:J:35:PHE:HD1	3:J:101:ARG:HB3	1.84	0.42
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.51	0.42
1:B:102:LEU:HA	1:B:102:LEU:HD23	1.82	0.42
2:C:239:MET:O	2:C:284:LEU:HD12	2.19	0.42
2:C:615:VAL:HG13	2:C:651:ASP:H	1.84	0.42
5:F:582:VAL:HG12	5:F:586:ARG:HG2	2.01	0.42
2:I:555:TYR:CD2	6:I:1401:42S:H1	2.55	0.42
2:I:816:ILE:HG22	2:I:818:VAL:HG23	2.00	0.42
3:J:45:ASN:HB3	3:J:48:THR:O	2.19	0.42
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.71	0.42
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.99	0.42
3:J:599:LYS:HD3	3:J:599:LYS:HA	1.75	0.42
3:J:797:THR:O	3:J:801:VAL:HG13	2.19	0.42
3:J:806:ASP:O	3:J:808:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.84	0.42
3:J:1259:GLN:NE2	3:J:1262:ARG:HH12	2.17	0.42
2:C:696:ASP:O	2:C:697:LYS:HB3	2.19	0.42
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.54	0.42
3:J:1174:ARG:HG2	3:J:1189:MET:SD	2.59	0.42
5:L:139:GLU:HG2	5:L:351:THR:HA	2.01	0.42
3:D:362:ARG:H	3:D:365:GLN:NE2	2.18	0.42
3:D:646:ILE:H	3:D:646:ILE:HG12	1.59	0.42
3:D:1172:LYS:HA	3:D:1191:PRO:HA	2.02	0.42
5:F:575:GLU:O	5:F:579:GLN:HG2	2.18	0.42
1:G:49:SER:OG	1:G:50:SER:N	2.53	0.42
1:H:48:LEU:HD21	3:J:535:ARG:HG3	2.01	0.42
2:I:518:ASN:O	2:I:691:PRO:HD3	2.19	0.42
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	2.01	0.42
1:A:231:PHE:HB3	1:B:218:ARG:HH11	1.84	0.42
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.54	0.42
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	2.02	0.42
3:D:94:GLN:O	3:D:97:VAL:HG23	2.20	0.42
1:G:145:LYS:HE3	1:G:145:LYS:HB3	1.79	0.42
1:H:67:GLU:O	1:H:78:ILE:HB	2.20	0.42
2:I:83:GLN:O	2:I:87:ILE:HG13	2.18	0.42
2:I:615:VAL:HG13	2:I:651:ASP:H	1.83	0.42
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.82	0.42
3:J:1314:LEU:HD11	3:J:1330:ARG:HH22	1.83	0.42
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.49	0.42
5:L:227:GLN:HG2	5:L:252:LEU:HA	2.02	0.42
1:A:113:ALA:HB2	1:A:126:PRO:HB3	2.01	0.42
1:B:11:PRO:HB3	1:B:30:PRO:O	2.20	0.42
1:B:82:LEU:HD23	1:B:85:LEU:HD12	2.01	0.42
2:C:1085:MET:HE2	2:C:1085:MET:HA	2.00	0.42
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.35	0.42
3:D:1174:ARG:HG2	3:D:1189:MET:SD	2.59	0.42
3:J:122:SER:O	3:J:126:LEU:HG	2.19	0.42
3:J:807:LEU:HD23	3:J:915:ILE:HG13	2.02	0.42
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.84	0.42
5:L:287:ILE:HG12	5:L:337:VAL:HG13	2.02	0.42
5:L:561:MET:HG2	5:L:576:VAL:HG22	2.02	0.42
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.27	0.42
2:C:120:GLN:HE21	2:C:120:GLN:HB2	1.57	0.42
2:C:700:VAL:HG11	2:C:1114:GLU:HG2	2.01	0.42
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:682:VAL:HA	3:D:685:ILE:HD13	2.01	0.42
5:F:571:TYR:HD1	5:F:575:GLU:HG2	1.82	0.42
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.27	0.42
2:I:696:ASP:O	2:I:697:LYS:HB3	2.20	0.42
2:I:739:ASP:OD1	2:I:739:ASP:N	2.53	0.42
2:I:1100:PRO:O	2:I:1104:PRO:HD3	2.20	0.42
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.19	0.42
3:J:1172:LYS:HA	3:J:1191:PRO:HA	2.01	0.42
5:L:250:LEU:O	5:L:254:GLU:HG2	2.19	0.42
1:A:99:ILE:HG12	1:A:145:LYS:HG2	2.02	0.42
1:A:207:THR:HG22	1:A:209:GLY:H	1.83	0.42
1:A:228:LEU:HD13	1:A:228:LEU:HA	1.78	0.42
1:B:81:ILE:O	1:B:85:LEU:HG	2.20	0.42
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.87	0.42
2:C:696:ASP:HB3	2:C:697:LYS:H	1.64	0.42
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.67	0.42
2:C:730:SER:O	2:C:753:LEU:HB2	2.19	0.42
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	2.01	0.42
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.19	0.42
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.54	0.42
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.93	0.42
5:F:227:GLN:HG2	5:F:252:LEU:HA	2.02	0.42
2:I:117:ILE:HD12	2:I:488:MET:HG2	2.01	0.42
2:I:183:TRP:HB2	2:I:199:ASP:HA	2.02	0.42
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.54	0.42
2:I:661:VAL:HB	2:I:665:ALA:HB3	2.01	0.42
2:I:1007:LYS:O	2:I:1011:LEU:HG	2.18	0.42
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.55	0.42
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.01	0.42
3:J:515:ARG:HH21	3:J:717:VAL:HG23	1.85	0.42
3:J:976:THR:HA	3:J:999:TYR:HE1	1.84	0.42
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.55	0.42
3:D:347:VAL:HG12	3:D:348:ASP:O	2.20	0.42
3:D:1295:ASN:HA	3:J:1206:ARG:NH2	2.35	0.42
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.89	0.42
1:H:82:LEU:HD23	1:H:85:LEU:HD12	2.01	0.42
2:I:23:ASP:OD1	2:I:23:ASP:N	2.48	0.42
2:I:169:LYS:O	2:I:169:LYS:HG2	2.19	0.42
3:J:198:CYS:HA	3:J:221:ILE:HD13	2.02	0.42
2:C:518:ASN:O	2:C:691:PRO:HD3	2.20	0.42
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:198:CYS:HA	3:D:221:ILE:HD13	2.02	0.42
5:F:139:GLU:HG2	5:F:351:THR:HA	2.01	0.42
5:F:528:LEU:HD23	5:F:528:LEU:HA	1.93	0.42
2:I:356:THR:HG21	2:I:362:ALA:HA	2.02	0.42
2:I:700:VAL:HG11	2:I:1114:GLU:HG2	2.01	0.42
3:J:156:ARG:NH2	3:J:191:SER:OG	2.52	0.42
5:L:565:ILE:HG22	5:L:566:ASP:CG	2.45	0.42
2:C:27:LEU:O	2:C:528:ARG:NH1	2.45	0.41
2:C:178:PRO:HB3	2:C:395:TYR:CZ	2.55	0.41
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.55	0.41
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.55	0.41
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	2.02	0.41
2:I:62:TYR:C	2:I:64:GLY:H	2.27	0.41
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.55	0.41
3:J:384:LYS:HD2	3:J:387:LEU:HD23	2.02	0.41
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.35	0.41
3:J:1241:TYR:HD2	3:J:1246:VAL:HG11	1.85	0.41
5:L:528:LEU:HD23	5:L:528:LEU:HA	1.96	0.41
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.89	0.41
1:A:61:ILE:HG23	1:A:142:MET:HB3	2.01	0.41
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.20	0.41
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.48	0.41
1:G:99:ILE:HG12	1:G:145:LYS:HG2	2.01	0.41
1:G:113:ALA:HB2	1:G:126:PRO:HB3	2.01	0.41
1:H:51:MET:HB3	1:H:178:SER:HA	2.02	0.41
5:L:598:LEU:O	5:L:604:SER:OG	2.36	0.41
2:C:102:LEU:HB2	2:C:489:PRO:HG3	2.02	0.41
2:C:138:ILE:HG22	2:C:139:ASN:N	2.34	0.41
2:C:555:TYR:CD2	6:C:1401:42S:H1	2.54	0.41
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.77	0.41
3:D:214:ARG:HA	3:D:217:LEU:HB2	2.02	0.41
1:H:81:ILE:O	1:H:85:LEU:HG	2.20	0.41
2:I:102:LEU:HB2	2:I:489:PRO:HG3	2.02	0.41
3:J:709:ARG:HA	3:J:709:ARG:HD2	1.92	0.41
3:J:976:THR:HA	3:J:999:TYR:CE1	2.55	0.41
5:L:559:LEU:HD12	5:L:559:LEU:HA	1.83	0.41
1:B:178:SER:HA	1:B:179:PRO:HD3	1.90	0.41
2:C:538:LEU:H	2:C:538:LEU:HG	1.69	0.41
2:C:867:GLU:H	2:C:867:GLU:HG3	1.62	0.41
4:E:35:LYS:NZ	4:E:71:GLU:OE2	2.49	0.41
5:F:457:ILE:HA	5:F:460:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:13:LYS:NZ	2:I:1151:LEU:HB2	2.36	0.41
2:I:587:LEU:HD23	2:I:587:LEU:HA	1.89	0.41
2:I:840:SER:HB2	2:I:850:ILE:HD11	2.03	0.41
2:I:867:GLU:H	2:I:867:GLU:HG3	1.61	0.41
5:L:96:ASP:O	5:L:98:VAL:N	2.53	0.41
5:L:601:PRO:HB3	5:L:604:SER:HB2	2.02	0.41
1:A:42:ALA:O	1:A:46:ILE:HG12	2.21	0.41
1:A:115:ILE:HG22	1:A:116:THR:H	1.86	0.41
2:C:734:ILE:HD12	2:C:777:VAL:HG21	2.03	0.41
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.01	0.41
3:D:741:ALA:O	3:D:762:ASN:ND2	2.54	0.41
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.21	0.41
4:E:8:ASP:O	4:E:11:GLU:HB2	2.21	0.41
1:G:228:LEU:HD13	1:G:228:LEU:HA	1.80	0.41
1:H:102:LEU:HA	1:H:102:LEU:HD23	1.82	0.41
2:I:734:ILE:HD12	2:I:777:VAL:HG21	2.01	0.41
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.03	0.41
1:B:134:THR:HG23	1:B:135:ASP:H	1.86	0.41
2:C:55:SER:OG	2:C:56:VAL:N	2.52	0.41
2:C:62:TYR:C	2:C:64:GLY:H	2.28	0.41
2:C:589:THR:HA	2:C:590:PRO:HD3	1.93	0.41
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	2.03	0.41
3:D:384:LYS:HD2	3:D:387:LEU:HD23	2.02	0.41
3:D:832:LYS:HD3	3:D:1242:ARG:NH1	2.35	0.41
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.85	0.41
5:F:134:VAL:HG21	5:F:266:PHE:CE1	2.45	0.41
5:F:503:GLU:CD	5:F:504:PRO:HD2	2.45	0.41
5:F:533:ASP:O	5:F:536:THR:N	2.53	0.41
1:G:77:ASP:O	1:G:81:ILE:HG13	2.20	0.41
2:I:466:VAL:O	2:I:469:VAL:HG22	2.21	0.41
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.61	0.41
3:J:557:LYS:HE3	3:J:557:LYS:HB2	1.79	0.41
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.21	0.41
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.21	0.41
5:L:457:ILE:HA	5:L:460:ILE:HD12	2.02	0.41
2:C:237:LEU:HD13	2:C:237:LEU:HA	1.82	0.41
2:C:801:ARG:HD3	2:C:1094:VAL:HA	2.03	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.82	0.41
3:D:461:PHE:HD2	3:D:461:PHE:HA	1.75	0.41
3:D:885:VAL:HG12	3:D:894:VAL:HG11	2.03	0.41
5:F:312:SER:OG	5:F:313:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	2.01	0.41
2:I:81:ASP:O	2:I:85:CYS:HB2	2.20	0.41
2:I:178:PRO:HB3	2:I:395:TYR:CZ	2.55	0.41
2:I:503:LYS:HD2	2:I:503:LYS:HA	1.89	0.41
3:J:356:THR:OG1	3:J:357:VAL:N	2.48	0.41
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.01	0.41
2:C:42:ASP:HA	2:C:43:PRO:HD3	1.87	0.41
2:C:60:GLN:H	2:C:60:GLN:HG2	1.74	0.41
2:C:143:ARG:NH2	2:C:507:GLY:O	2.53	0.41
2:C:582:ASN:HB3	2:C:586:PHE:N	2.34	0.41
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.56	0.41
3:D:35:PHE:HD1	3:D:101:ARG:HB3	1.85	0.41
3:D:62:PHE:O	3:D:101:ARG:HD2	2.21	0.41
3:D:839:VAL:HG13	3:D:882:VAL:HG21	2.02	0.41
3:D:931:THR:OG1	3:D:1244:GLN:NE2	2.54	0.41
1:H:147:GLN:HG3	1:H:148:ARG:H	1.86	0.41
2:I:151:ARG:CZ	2:I:445:ILE:HD11	2.51	0.41
2:I:299:LYS:HB3	2:I:299:LYS:HE2	1.95	0.41
2:I:974:ARG:HB3	2:I:1014:LEU:HD21	2.03	0.41
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.21	0.41
3:J:396:ALA:O	3:J:400:MET:HG3	2.21	0.41
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.70	0.41
5:L:517:SER:O	5:L:518:HIS:HD2	2.04	0.41
2:C:208:ILE:HD11	2:C:365:GLU:HB3	2.03	0.41
3:D:45:ASN:HB3	3:D:48:THR:O	2.21	0.41
3:D:343:LEU:HD12	3:D:343:LEU:HA	1.81	0.41
3:D:527:LEU:HB2	3:D:550:VAL:HG12	2.02	0.41
3:D:701:LEU:HD13	3:D:723:TYR:HB2	2.03	0.41
3:D:709:ARG:HA	3:D:709:ARG:HD2	1.92	0.41
3:D:850:LYS:HB3	3:D:851:PRO:HD2	2.02	0.41
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.87	0.41
3:D:1259:GLN:NE2	3:D:1262:ARG:HH12	2.18	0.41
3:D:1372:ARG:HE	3:J:854:ALA:HB2	1.85	0.41
5:F:96:ASP:O	5:F:98:VAL:N	2.54	0.41
5:F:161:LEU:HD12	5:F:161:LEU:HA	1.92	0.41
5:F:234:THR:O	5:F:245:ALA:HB2	2.21	0.41
5:F:250:LEU:O	5:F:254:GLU:HG2	2.21	0.41
5:F:296:LYS:HA	5:F:296:LYS:HD3	1.78	0.41
5:F:343:LYS:O	5:F:347:ILE:HG13	2.21	0.41
5:F:601:PRO:HB3	5:F:604:SER:HB2	2.03	0.41
1:G:42:ALA:O	1:G:46:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:61:ILE:HG22	1:G:62:ASP:H	1.85	0.41
1:H:19:VAL:HB	1:H:23:HIS:HD2	1.85	0.41
1:H:61:ILE:HB	1:H:64:VAL:O	2.21	0.41
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	2.03	0.41
3:J:294:ASN:HD22	5:L:406:GLN:HE21	1.69	0.41
3:J:793:SER:O	3:J:797:THR:HG23	2.21	0.41
3:J:839:VAL:HG13	3:J:882:VAL:HG21	2.01	0.41
3:J:850:LYS:HB3	3:J:851:PRO:HD2	2.02	0.41
5:L:476:ARG:HG3	5:L:477:GLU:N	2.34	0.41
5:L:512:GLY:C	5:L:514:ASP:H	2.29	0.41
1:A:228:LEU:HD21	1:B:224:LEU:HD23	2.03	0.41
2:C:13:LYS:NZ	2:C:1151:LEU:HB2	2.36	0.41
2:C:137:VAL:HA	2:C:141:THR:O	2.21	0.41
2:C:169:LYS:O	2:C:169:LYS:HG2	2.20	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.02	0.41
2:C:1124:ILE:HB	2:C:1180:MET:HB2	2.03	0.41
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.86	0.41
3:D:122:SER:O	3:D:126:LEU:HG	2.20	0.41
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.03	0.41
2:I:208:ILE:HD11	2:I:365:GLU:HB3	2.03	0.41
3:J:214:ARG:HA	3:J:217:LEU:HB2	2.03	0.41
3:J:325:LYS:HG3	3:J:329:ASP:HB2	2.03	0.41
3:J:664:ILE:HG22	3:J:678:ARG:HG2	2.03	0.41
5:L:387:VAL:HG22	5:L:435:ILE:HD13	2.03	0.41
1:A:90:VAL:HG22	1:A:91:ARG:H	1.86	0.40
3:D:451:PRO:O	3:D:454:CYS:HB2	2.21	0.40
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.89	0.40
1:G:61:ILE:HG23	1:G:142:MET:HB3	2.02	0.40
2:I:127:ILE:HA	2:I:128:PRO:HD3	1.92	0.40
3:J:347:VAL:HG12	3:J:348:ASP:O	2.22	0.40
3:J:491:LEU:HD22	3:J:496:GLY:O	2.21	0.40
3:J:832:LYS:HD3	3:J:1242:ARG:NH1	2.36	0.40
5:L:312:SER:OG	5:L:313:ASP:N	2.54	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.50	0.40
1:B:61:ILE:HB	1:B:64:VAL:O	2.21	0.40
2:C:299:LYS:HB3	2:C:299:LYS:HE2	1.96	0.40
2:C:791:LEU:HD23	2:C:791:LEU:HA	1.90	0.40
3:D:57:PHE:HB3	3:D:98:ARG:HH22	1.86	0.40
3:D:233:LYS:HA	3:D:234:PRO:HD3	1.94	0.40
3:D:474:LEU:HA	3:D:477:GLN:HG3	2.03	0.40
4:E:15:ASN:O	4:E:16:ARG:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:ARG:HB3	1:H:198:LEU:HD21	2.03	0.40
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	2.02	0.40
3:J:527:LEU:HB2	3:J:550:VAL:HG12	2.02	0.40
3:J:833:GLU:HA	3:J:834:PRO:HD3	1.85	0.40
3:J:931:THR:OG1	3:J:1244:GLN:NE2	2.54	0.40
5:L:137:TYR:CD2	5:L:273:MET:HE2	2.56	0.40
5:L:604:SER:O	5:L:608:ARG:HB2	2.21	0.40
1:B:205:MET:HE3	1:B:213:PRO:HB3	2.03	0.40
2:C:860:ALA:O	2:C:863:SER:OG	2.34	0.40
2:C:1101:LEU:HD12	3:D:505:ASP:OD2	2.22	0.40
3:D:262:THR:C	5:F:507:MET:HB2	2.45	0.40
3:D:1198:VAL:HB	3:D:1210:ILE:HA	2.04	0.40
1:G:212:ASP:HA	1:G:213:PRO:HD3	1.97	0.40
1:H:134:THR:HG23	1:H:135:ASP:H	1.86	0.40
2:I:175:ARG:HD3	2:I:183:TRP:CZ3	2.56	0.40
2:I:1092:THR:HA	2:I:1093:PRO:HD3	1.96	0.40
2:I:1164:PHE:O	2:I:1169:VAL:HG23	2.21	0.40
3:J:362:ARG:H	3:J:365:GLN:NE2	2.18	0.40
3:J:972:LYS:HB3	3:J:1002:VAL:HG13	2.03	0.40
4:K:10:VAL:HG13	4:K:16:ARG:HB2	2.02	0.40
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.33	0.40
5:L:470:MET:HE3	5:L:470:MET:HB3	2.01	0.40
2:C:175:ARG:HD3	2:C:183:TRP:CZ3	2.57	0.40
3:D:683:ILE:HD11	3:D:754:ILE:HG12	2.03	0.40
5:F:565:ILE:HG22	5:F:566:ASP:CG	2.46	0.40
5:F:572:THR:O	5:F:576:VAL:HG23	2.20	0.40
1:H:205:MET:HE3	1:H:213:PRO:HB3	2.04	0.40
2:I:11:ILE:HD13	2:I:11:ILE:HA	1.93	0.40
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.93	0.40
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.86	0.40
1:B:147:GLN:HG3	1:B:148:ARG:H	1.86	0.40
2:C:59:ILE:HD13	2:C:472:GLU:HA	2.04	0.40
2:C:379:GLU:H	2:C:379:GLU:CD	2.29	0.40
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.92	0.40
2:C:739:ASP:OD1	2:C:739:ASP:N	2.52	0.40
2:C:840:SER:HB2	2:C:850:ILE:HD11	2.02	0.40
3:D:367:GLY:HA3	3:D:448:GLN:HB2	2.03	0.40
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.79	0.40
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.21	0.40
3:D:609:TYR:HB2	3:D:617:THR:HG21	2.04	0.40
5:F:287:ILE:HG12	5:F:337:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:GLY:O	1:H:134:THR:N	2.42	0.40
2:I:972:PHE:HB2	2:I:994:ARG:HH21	1.87	0.40
3:J:22:ILE:O	3:J:1339:GLY:HA2	2.21	0.40
3:J:110:PRO:HD2	3:J:183:GLU:HG2	2.04	0.40
3:J:741:ALA:O	3:J:762:ASN:ND2	2.54	0.40
5:L:315:TRP:CZ2	5:L:341:LEU:HD21	2.55	0.40
5:L:397:ARG:HG2	5:L:443:ILE:HG21	2.03	0.40
5:L:551:LEU:HD21	5:L:598:LEU:HD21	2.02	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	222/239 (93%)	191 (86%)	28 (13%)	3 (1%)	9	37
1	B	216/239 (90%)	193 (89%)	23 (11%)	0	100	100
1	G	226/239 (95%)	196 (87%)	27 (12%)	3 (1%)	9	38
1	H	213/239 (89%)	193 (91%)	20 (9%)	0	100	100
2	C	1338/1342 (100%)	1231 (92%)	102 (8%)	5 (0%)	30	60
2	I	1338/1342 (100%)	1230 (92%)	103 (8%)	5 (0%)	30	60
3	D	1162/1407 (83%)	1075 (92%)	83 (7%)	4 (0%)	36	65
3	J	1230/1407 (87%)	1141 (93%)	84 (7%)	5 (0%)	30	60
4	E	87/91 (96%)	80 (92%)	7 (8%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	464/522 (89%)	423 (91%)	40 (9%)	1 (0%)	43	72
5	L	463/522 (89%)	420 (91%)	42 (9%)	1 (0%)	43	72
All	All	7036/7680 (92%)	6446 (92%)	563 (8%)	27 (0%)	30	60

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1159	VAL
2	I	1159	VAL
2	C	170	VAL
2	I	170	VAL
3	J	340	GLN
2	C	697	LYS
2	I	697	LYS
1	A	14	VAL
1	A	62	ASP
1	A	167	PRO
3	D	710	ASP
1	G	14	VAL
1	G	62	ASP
1	G	167	PRO
2	I	484	LEU
3	J	710	ASP
2	C	484	LEU
3	D	831	VAL
3	J	831	VAL
5	L	477	GLU
5	F	477	GLU
2	C	1186	VAL
2	I	1186	VAL
3	D	826	ILE
3	D	1180	VAL
3	J	826	ILE
3	J	1180	VAL

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	191/206 (93%)	175 (92%)	16 (8%)	10	35
1	B	184/206 (89%)	162 (88%)	22 (12%)	5	23
1	G	191/206 (93%)	175 (92%)	16 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	183/206 (89%)	164 (90%)	19 (10%)	7	28
2	C	1155/1157 (100%)	1040 (90%)	115 (10%)	7	30
2	I	1154/1157 (100%)	1041 (90%)	113 (10%)	7	30
3	D	975/1168 (84%)	863 (88%)	112 (12%)	5	24
3	J	1036/1168 (89%)	915 (88%)	121 (12%)	5	24
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	25
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	39
5	F	417/462 (90%)	375 (90%)	42 (10%)	7	29
5	L	418/462 (90%)	375 (90%)	43 (10%)	7	29
All	All	6043/6548 (92%)	5411 (90%)	632 (10%)	6	28

All (632) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	VAL
1	A	26	VAL
1	A	50	SER
1	A	61	ILE
1	A	64	VAL
1	A	74	VAL
1	A	115	ILE
1	A	129	VAL
1	A	133	LEU
1	A	158	ARG
1	A	165	GLU
1	A	215	GLU
1	A	219	ARG
1	A	228	LEU
1	A	231	PHE
1	B	6	THR
1	B	7	GLU
1	B	8	PHE
1	B	18	GLN
1	B	27	THR
1	B	29	GLU
1	B	50	SER
1	B	58	GLU
1	B	60	GLU

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Mol	Chain	Res	Type
1	B	64	VAL
1	B	65	LEU
1	B	75	GLN
1	B	80	GLU
1	B	97	GLU
1	B	107	ILE
1	B	110	VAL
1	B	124	VAL
1	B	133	LEU
1	B	134	THR
1	B	160	HIS
1	B	183	ILE
1	B	193	GLU
2	C	4	SER
2	C	11	ILE
2	C	21	VAL
2	C	22	LEU
2	C	39	ILE
2	C	60	GLN
2	C	82	VAL
2	C	85	CYS
2	C	90	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	132	ASP
2	C	167	SER
2	C	170	VAL
2	C	237	LEU
2	C	285	ILE
2	C	292	ILE
2	C	299	LYS
2	C	302	ILE
2	C	306	THR
2	C	320	ASP
2	C	321	LEU
2	C	353	VAL

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Mol	Chain	Res	Type
2	C	360	LEU
2	C	377	THR
2	C	379	GLU
2	C	394	ARG
2	C	400	VAL
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	445	ILE
2	C	453	ILE
2	C	484	LEU
2	C	486	THR
2	C	490	GLN
2	C	493	ILE
2	C	503	LYS
2	C	538	LEU
2	C	539	THR
2	C	542	ARG
2	C	550	VAL
2	C	558	VAL
2	C	565	GLU
2	C	589	THR
2	C	604	HIS
2	C	607	SER
2	C	609	ILE
2	C	615	VAL
2	C	620	ASN
2	C	623	LEU
2	C	633	LEU
2	C	639	LYS
2	C	657	THR
2	C	672	GLU
2	C	680	LEU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	781	ASP
2	C	788	SER

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Mol	Chain	Res	Type
2	C	800	MET
2	C	817	LEU
2	C	819	SER
2	C	826	ASP
2	C	840	SER
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	1002	LEU
2	C	1040	ASP
2	C	1046	VAL
2	C	1073	LYS
2	C	1082	ILE
2	C	1083	GLU
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1146	GLN
2	C	1151	LEU
2	C	1156	ARG
2	C	1159	VAL
2	C	1161	LEU
2	C	1174	GLU
2	C	1180	MET
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1238	LEU
2	C	1254	VAL
2	C	1264	GLN
2	C	1293	VAL
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1340	GLU

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Mol	Chain	Res	Type
2	C	1341	ASP
2	C	1342	GLU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE
3	D	26	SER
3	D	46	TYR
3	D	79	LYS
3	D	83	VAL
3	D	84	ILE
3	D	92	VAL
3	D	94	GLN
3	D	95	THR
3	D	97	VAL
3	D	106	GLU
3	D	159	ILE
3	D	169	LEU
3	D	175	GLU
3	D	217	LEU
3	D	244	VAL
3	D	252	LEU
3	D	255	LEU
3	D	256	ASP
3	D	299	LEU
3	D	306	LEU
3	D	312	ARG
3	D	324	LEU
3	D	330	MET
3	D	334	LYS
3	D	363	LEU
3	D	374	LEU
3	D	394	ILE
3	D	401	VAL
3	D	416	ILE
3	D	425	ARG
3	D	429	LEU
3	D	454	CYS
3	D	490	ILE
3	D	501	VAL
3	D	506	VAL
3	D	507	VAL
3	D	510	LEU

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Mol	Chain	Res	Type
3	D	513	MET
3	D	514	THR
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	568	SER
3	D	573	THR
3	D	594	GLN
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL
3	D	678	ARG
3	D	680	ASN
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	740	LEU
3	D	746	LEU
3	D	754	ILE
3	D	769	VAL
3	D	770	LEU
3	D	788	LEU
3	D	798	ARG
3	D	803	VAL
3	D	810	THR
3	D	826	ILE
3	D	844	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR

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Mol	Chain	Res	Type
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	881	LYS
3	D	897	HIS
3	D	908	ILE
3	D	918	ILE
3	D	1155	ILE
3	D	1163	VAL
3	D	1170	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1194	ARG
3	D	1202	GLU
3	D	1221	LEU
3	D	1255	VAL
3	D	1268	ASN
3	D	1273	ASP
3	D	1274	PHE
3	D	1275	LEU
3	D	1278	GLU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1310	THR
3	D	1333	THR
3	D	1343	GLU
4	E	5	THR
4	E	13	ILE
4	E	16	ARG
4	E	21	LEU
4	E	28	ARG
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	127	ILE

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Mol	Chain	Res	Type
5	F	130	VAL
5	F	154	GLU
5	F	247	GLU
5	F	267	ASP
5	F	297	MET
5	F	301	ASN
5	F	305	LEU
5	F	306	PHE
5	F	310	GLU
5	F	341	LEU
5	F	395	THR
5	F	400	GLN
5	F	429	THR
5	F	437	GLN
5	F	449	THR
5	F	450	ILE
5	F	471	LEU
5	F	472	GLN
5	F	479	THR
5	F	482	GLU
5	F	485	GLU
5	F	486	ARG
5	F	488	LEU
5	F	489	MET
5	F	494	ILE
5	F	508	GLU
5	F	530	LEU
5	F	547	VAL
5	F	558	VAL
5	F	561	MET
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	580	PHE
5	F	587	ILE
5	F	603	ARG
5	F	606	VAL
5	F	612	ASP
1	G	9	LEU
1	G	19	VAL
1	G	26	VAL
1	G	50	SER

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Mol	Chain	Res	Type
1	G	61	ILE
1	G	64	VAL
1	G	74	VAL
1	G	115	ILE
1	G	129	VAL
1	G	133	LEU
1	G	158	ARG
1	G	165	GLU
1	G	215	GLU
1	G	219	ARG
1	G	228	LEU
1	G	231	PHE
1	H	6	THR
1	H	18	GLN
1	H	27	THR
1	H	29	GLU
1	H	50	SER
1	H	58	GLU
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	80	GLU
1	H	97	GLU
1	H	107	ILE
1	H	110	VAL
1	H	124	VAL
1	H	133	LEU
1	H	134	THR
1	H	183	ILE
1	H	193	GLU
2	I	4	SER
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	60	GLN
2	I	82	VAL
2	I	85	CYS
2	I	90	VAL
2	I	91	THR
2	I	115	LYS
2	I	116	ASP

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Mol	Chain	Res	Type
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	132	ASP
2	I	167	SER
2	I	170	VAL
2	I	237	LEU
2	I	285	ILE
2	I	292	ILE
2	I	299	LYS
2	I	302	ILE
2	I	306	THR
2	I	320	ASP
2	I	321	LEU
2	I	353	VAL
2	I	360	LEU
2	I	377	THR
2	I	379	GLU
2	I	394	ARG
2	I	400	VAL
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	445	ILE
2	I	453	ILE
2	I	484	LEU
2	I	486	THR
2	I	490	GLN
2	I	493	ILE
2	I	503	LYS
2	I	538	LEU
2	I	539	THR
2	I	542	ARG
2	I	550	VAL
2	I	558	VAL
2	I	565	GLU
2	I	589	THR
2	I	600	THR
2	I	604	HIS
2	I	607	SER
2	I	609	ILE

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Mol	Chain	Res	Type
2	I	615	VAL
2	I	620	ASN
2	I	623	LEU
2	I	633	LEU
2	I	639	LYS
2	I	672	GLU
2	I	680	LEU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	788	SER
2	I	800	MET
2	I	817	LEU
2	I	819	SER
2	I	826	ASP
2	I	840	SER
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	979	LEU
2	I	984	VAL
2	I	1002	LEU
2	I	1040	ASP
2	I	1046	VAL
2	I	1073	LYS
2	I	1082	ILE
2	I	1083	GLU
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1146	GLN
2	I	1151	LEU

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Mol	Chain	Res	Type
2	I	1156	ARG
2	I	1159	VAL
2	I	1161	LEU
2	I	1174	GLU
2	I	1180	MET
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1238	LEU
2	I	1254	VAL
2	I	1264	GLN
2	I	1293	VAL
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1340	GLU
2	I	1341	ASP
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	26	SER
3	J	46	TYR
3	J	79	LYS
3	J	83	VAL
3	J	84	ILE
3	J	92	VAL
3	J	94	GLN
3	J	95	THR
3	J	97	VAL
3	J	106	GLU
3	J	159	ILE
3	J	169	LEU
3	J	175	GLU
3	J	217	LEU
3	J	244	VAL
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	299	LEU
3	J	306	LEU
3	J	312	ARG
3	J	324	LEU

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Mol	Chain	Res	Type
3	J	330	MET
3	J	334	LYS
3	J	363	LEU
3	J	374	LEU
3	J	394	ILE
3	J	401	VAL
3	J	416	ILE
3	J	425	ARG
3	J	429	LEU
3	J	454	CYS
3	J	490	ILE
3	J	501	VAL
3	J	506	VAL
3	J	507	VAL
3	J	510	LEU
3	J	513	MET
3	J	514	THR
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	568	SER
3	J	573	THR
3	J	594	GLN
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL
3	J	678	ARG
3	J	680	ASN
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN

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Mol	Chain	Res	Type
3	J	740	LEU
3	J	746	LEU
3	J	754	ILE
3	J	769	VAL
3	J	770	LEU
3	J	788	LEU
3	J	798	ARG
3	J	803	VAL
3	J	810	THR
3	J	826	ILE
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	881	LYS
3	J	897	HIS
3	J	908	ILE
3	J	918	ILE
3	J	960	LEU
3	J	963	VAL
3	J	972	LYS
3	J	987	GLU
3	J	992	LYS
3	J	994	SER
3	J	997	VAL
3	J	1010	GLN
3	J	1017	VAL
3	J	1027	VAL
3	J	1155	ILE
3	J	1163	VAL
3	J	1170	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1194	ARG
3	J	1202	GLU
3	J	1221	LEU
3	J	1255	VAL
3	J	1268	ASN

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Mol	Chain	Res	Type
3	J	1273	ASP
3	J	1274	PHE
3	J	1275	LEU
3	J	1278	GLU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1310	THR
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	21	LEU
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	130	VAL
5	L	154	GLU
5	L	247	GLU
5	L	267	ASP
5	L	297	MET
5	L	301	ASN
5	L	305	LEU
5	L	306	PHE
5	L	310	GLU
5	L	341	LEU
5	L	395	THR
5	L	400	GLN
5	L	429	THR
5	L	437	GLN
5	L	449	THR
5	L	450	ILE
5	L	471	LEU
5	L	472	GLN
5	L	479	THR
5	L	482	GLU
5	L	485	GLU

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Mol	Chain	Res	Type
5	L	486	ARG
5	L	488	LEU
5	L	489	MET
5	L	490	PRO
5	L	494	ILE
5	L	508	GLU
5	L	530	LEU
5	L	547	VAL
5	L	558	VAL
5	L	561	MET
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	580	PHE
5	L	587	ILE
5	L	603	ARG
5	L	606	VAL
5	L	612	ASP
5	L	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	103	ASN
1	A	117	HIS
1	A	132	HIS
1	B	75	GLN
1	B	84	ASN
1	B	137	ASN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	494	ASN
2	C	628	HIS
2	C	677	ASN
2	C	688	GLN
2	C	761	GLN
2	C	1061	GLN
2	C	1116	HIS
2	C	1136	GLN
2	C	1146	GLN

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Mol	Chain	Res	Type
2	C	1209	GLN
2	C	1237	HIS
2	C	1288	GLN
2	C	1313	HIS
2	C	1314	GLN
3	D	94	GLN
3	D	158	GLN
3	D	196	GLN
3	D	200	GLN
3	D	365	GLN
3	D	450	HIS
3	D	489	ASN
3	D	669	GLN
3	D	702	GLN
3	D	716	GLN
3	D	907	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1197	ASN
3	D	1218	HIS
3	D	1227	HIS
3	D	1244	GLN
3	D	1367	GLN
5	F	131	GLN
5	F	227	GLN
5	F	246	GLN
5	F	317	ASN
5	F	362	ASN
5	F	396	ASN
5	F	406	GLN
5	F	446	GLN
5	F	464	ASN
5	F	472	GLN
5	F	600	HIS
1	G	103	ASN
1	G	117	HIS
1	H	137	ASN
2	I	31	GLN
2	I	69	GLN
2	I	139	ASN
2	I	494	ASN
2	I	628	HIS

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Mol	Chain	Res	Type
2	I	677	ASN
2	I	688	GLN
2	I	761	GLN
2	I	1061	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1209	GLN
2	I	1237	HIS
2	I	1288	GLN
2	I	1314	GLN
3	J	94	GLN
3	J	158	GLN
3	J	196	GLN
3	J	200	GLN
3	J	365	GLN
3	J	450	HIS
3	J	489	ASN
3	J	669	GLN
3	J	702	GLN
3	J	716	GLN
3	J	861	ASN
3	J	910	ASN
3	J	929	GLN
3	J	962	ASN
3	J	1010	GLN
3	J	1197	ASN
3	J	1218	HIS
3	J	1244	GLN
3	J	1295	ASN
3	J	1367	GLN
4	K	61	ASN
5	L	131	GLN
5	L	227	GLN
5	L	246	GLN
5	L	301	ASN
5	L	317	ASN
5	L	362	ASN
5	L	396	ASN
5	L	406	GLN
5	L	446	GLN

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Mol	Chain	Res	Type
5	L	464	ASN
5	L	600	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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$
6	42S	C	1401	-	20,21,21	1.06	1 (5%)	27,29,29	1.67	6 (22%)
6	42S	I	1401	-	20,21,21	1.06	1 (5%)	27,29,29	1.67	6 (22%)

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
6	42S	C	1401	-	-	0/16/16/16	0/2/2/2
6	42S	I	1401	-	-	0/16/16/16	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	42S	O20-N19	-3.04	1.31	1.40
6	I	1401	42S	O20-N19	-3.03	1.31	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	1401	42S	N07-C08-N19	5.48	132.84	124.05
6	C	1401	42S	N07-C08-N19	5.44	132.78	124.05
6	I	1401	42S	C02-C03-C04	3.50	123.77	119.73
6	C	1401	42S	C02-C03-C04	3.27	123.49	119.73
6	C	1401	42S	C13-C12-C11	-2.68	118.03	120.75
6	I	1401	42S	C13-C12-C11	-2.57	118.14	120.75
6	C	1401	42S	C09-C08-N07	2.51	124.58	116.49
6	I	1401	42S	C09-C08-N07	2.48	124.50	116.49
6	C	1401	42S	C05-C04-C03	-2.45	115.80	119.04
6	I	1401	42S	C05-C04-C03	-2.29	116.01	119.04
6	C	1401	42S	C12-C11-C10	2.01	121.72	117.86
6	I	1401	42S	C12-C11-C10	2.01	121.72	117.86

There are no chirality outliers.

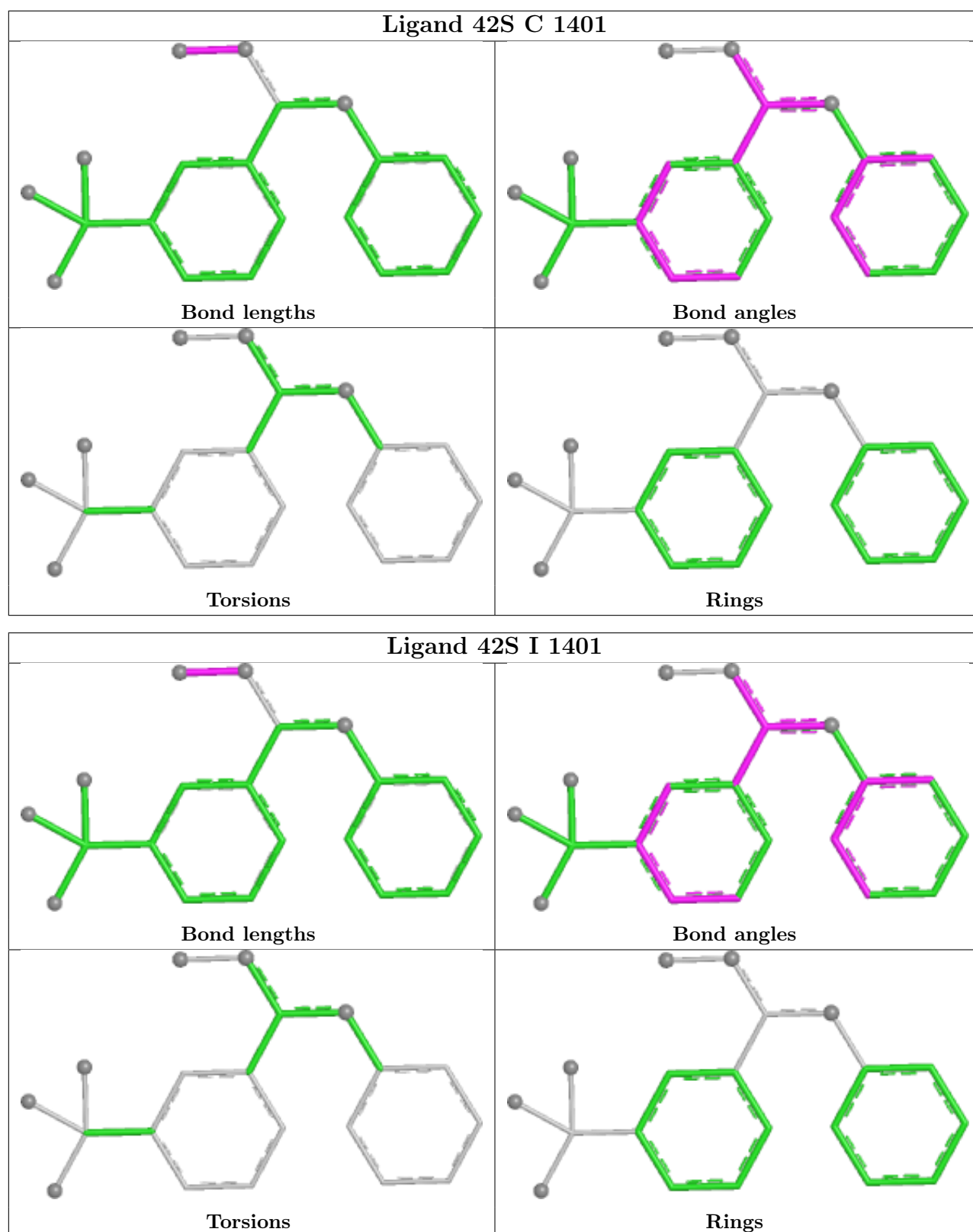
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1401	42S	2	0
6	I	1401	42S	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

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	224/239 (93%)	-0.62	1 (0%) 88 72	50, 88, 138, 174	0
1	B	220/239 (92%)	-0.23	7 (3%) 50 31	67, 131, 170, 190	0
1	G	228/239 (95%)	-0.47	0 100 100	77, 126, 157, 195	0
1	H	217/239 (90%)	-0.40	1 (0%) 87 69	88, 136, 160, 178	0
2	C	1340/1342 (99%)	-0.52	6 (0%) 88 72	29, 80, 138, 174	0
2	I	1340/1342 (99%)	-0.50	3 (0%) 91 80	45, 103, 155, 191	0
3	D	1166/1407 (82%)	-0.54	1 (0%) 92 86	26, 79, 150, 184	0
3	J	1236/1407 (87%)	-0.51	2 (0%) 91 80	42, 98, 154, 175	0
4	E	89/91 (97%)	-0.63	0 100 100	35, 78, 114, 130	0
4	K	79/91 (86%)	-0.60	0 100 100	62, 95, 151, 168	0
5	F	470/522 (90%)	-0.47	0 100 100	48, 119, 167, 189	0
5	L	469/522 (89%)	-0.44	0 100 100	59, 123, 167, 188	0
All	All	7078/7680 (92%)	-0.50	21 (0%) 90 76	26, 99, 157, 195	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	LEU	3.9
1	B	78	ILE	3.4
1	B	98	VAL	3.4
2	I	484	LEU	3.3
2	C	1000	LEU	3.2
2	C	929	ILE	2.9
1	B	146	VAL	2.7
1	A	225	ALA	2.6
2	C	606	LEU	2.4
3	J	522	GLY	2.3
1	B	82	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	1153	ALA	2.3
2	I	975	ILE	2.2
3	J	998	PRO	2.2
2	I	565	GLU	2.2
1	B	69	SER	2.1
2	C	999	GLU	2.1
1	B	81	ILE	2.1
2	C	483	ASP	2.0
1	H	234	LEU	2.0
3	D	1204	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

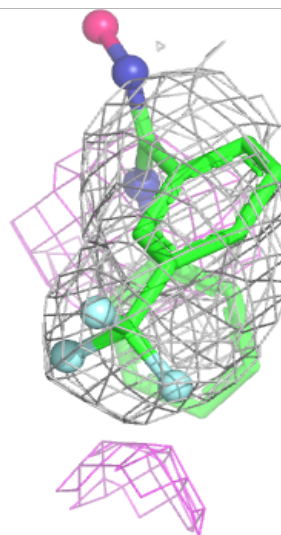
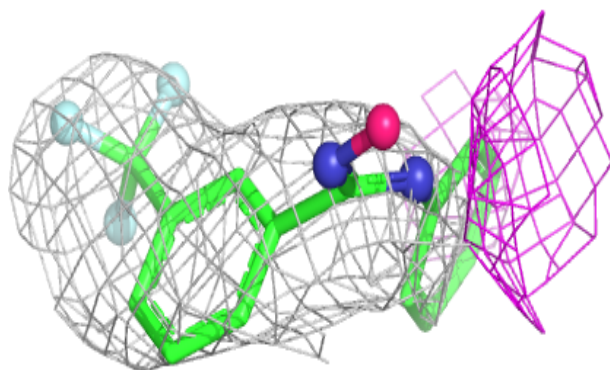
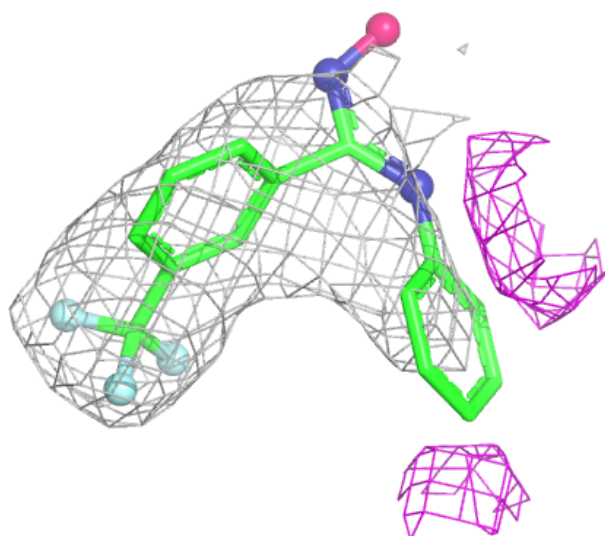
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

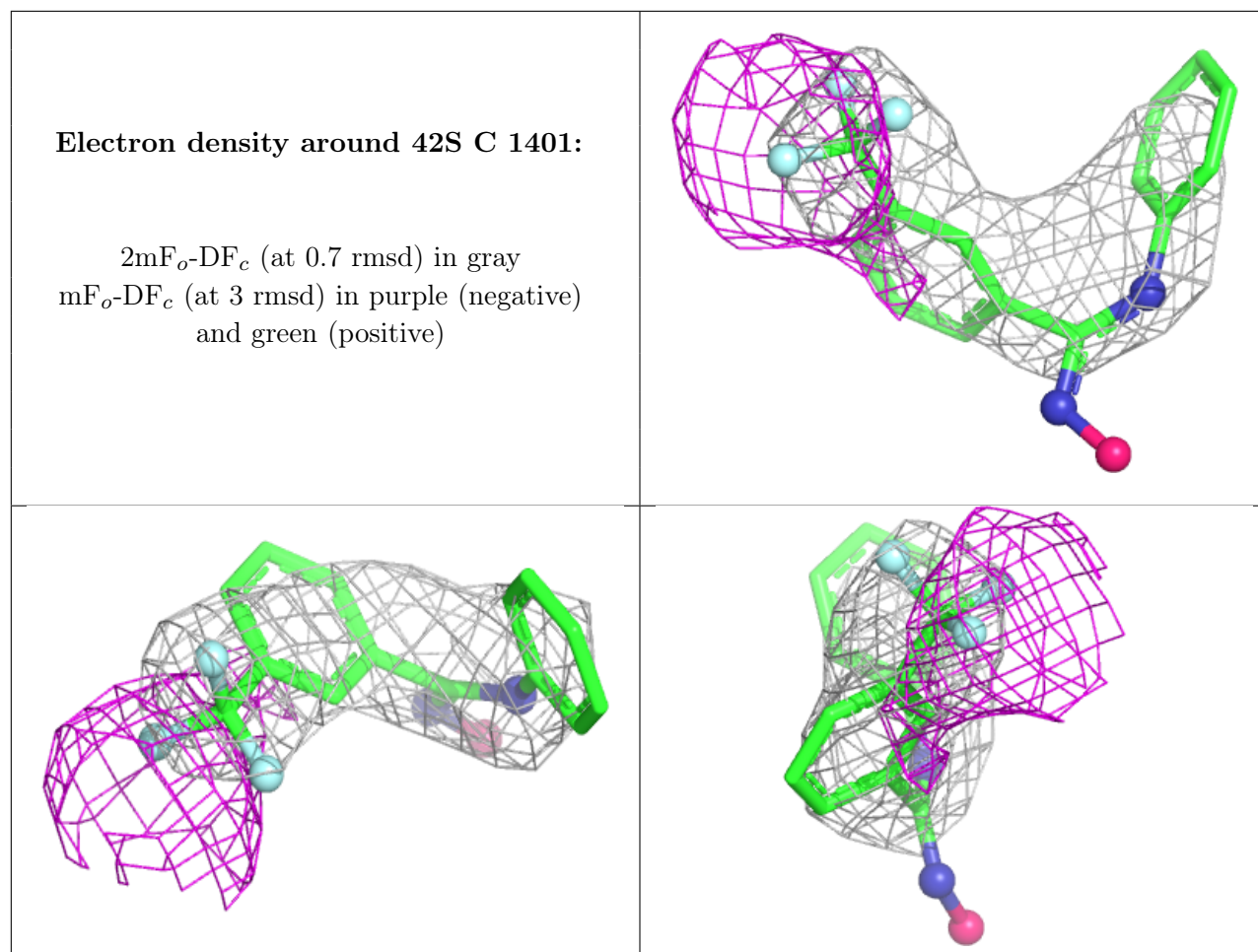
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	J	1501	1/1	0.71	0.08	82,82,82,82	0
8	ZN	J	1503	1/1	0.83	0.16	490,490,490,490	0
6	42S	I	1401	20/20	0.88	0.10	75,85,110,123	0
6	42S	C	1401	20/20	0.91	0.09	58,77,93,101	0
8	ZN	D	1503	1/1	0.93	0.14	420,420,420,420	0
8	ZN	D	1502	1/1	0.95	0.16	429,429,429,429	0
7	MG	D	1501	1/1	0.97	0.02	67,67,67,67	0
8	ZN	J	1502	1/1	0.99	0.10	199,199,199,199	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 42S I 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.