



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 11:40 AM UTC

PDB ID : 4ZH4 / pdb_00004zh4
Title : Crystal structure of Escherichia coli RNA polymerase in complex with CBRP18
Authors : Feng, Y.; Ebright, R.H.
Deposited on : 2015-04-24
Resolution : 3.99 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

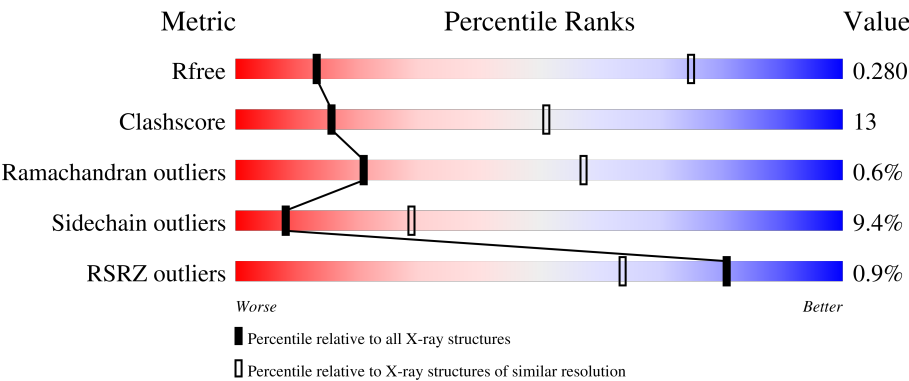
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.99 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	335	% 58%28%.10%
1	B	335	37%23%.36%
1	G	335	% 39%24%.33%
1	H	335	37%23%.36%
2	C	1342	% 65%31%.0%

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Mol	Chain	Length	Quality of chain
2	I	1342	% 67%29%.
3	D	1407	% 51%27%.18%
3	J	1407	59%31%.6%
4	E	91	73%23%. .
4	K	91	59%23%.13%
5	F	613	% 61%25%.12%
5	L	613	59%26%.12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 57539 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	302	Total	C	N	O	S	0	0	0
			2328	1456	413	451	8			
1	B	216	Total	C	N	O	S	0	0	0
			1667	1041	294	326	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P0A7Z4
A	-4	HIS	-	expression tag	UNP P0A7Z4
A	-3	HIS	-	expression tag	UNP P0A7Z4
A	-2	HIS	-	expression tag	UNP P0A7Z4
A	-1	HIS	-	expression tag	UNP P0A7Z4
A	0	HIS	-	expression tag	UNP P0A7Z4
A	1	HIS	-	expression tag	UNP P0A7Z4
B	-5	MET	-	expression tag	UNP P0A7Z4
B	-4	HIS	-	expression tag	UNP P0A7Z4
B	-3	HIS	-	expression tag	UNP P0A7Z4
B	-2	HIS	-	expression tag	UNP P0A7Z4
B	-1	HIS	-	expression tag	UNP P0A7Z4
B	0	HIS	-	expression tag	UNP P0A7Z4
B	1	HIS	-	expression tag	UNP P0A7Z4
G	-5	MET	-	expression tag	UNP P0A7Z4
G	-4	HIS	-	expression tag	UNP P0A7Z4
G	-3	HIS	-	expression tag	UNP P0A7Z4
G	-2	HIS	-	expression tag	UNP P0A7Z4
G	-1	HIS	-	expression tag	UNP P0A7Z4
G	0	HIS	-	expression tag	UNP P0A7Z4
G	1	HIS	-	expression tag	UNP P0A7Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	MET	-	expression tag	UNP P0A7Z4
H	-4	HIS	-	expression tag	UNP P0A7Z4
H	-3	HIS	-	expression tag	UNP P0A7Z4
H	-2	HIS	-	expression tag	UNP P0A7Z4
H	-1	HIS	-	expression tag	UNP P0A7Z4
H	0	HIS	-	expression tag	UNP P0A7Z4
H	1	HIS	-	expression tag	UNP P0A7Z4

- 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	1151	Total	C	N	O	S	0	0	0
			8992	5653	1608	1686	45			
3	J	1319	Total	C	N	O	S	0	0	0
			10254	6443	1824	1939	48			

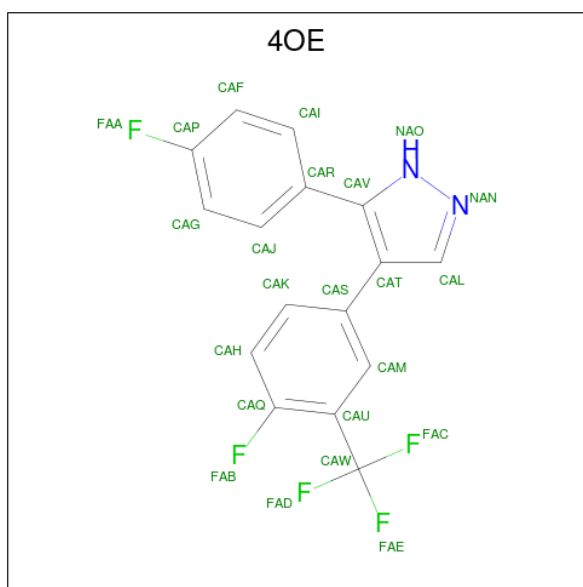
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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	542	Total	C	N	O	S	0	0	0
			4204	2625	752	801	26			
5	L	539	Total	C	N	O	S	0	0	0
			4196	2619	749	802	26			

- Molecule 6 is 5-(4-fluorophenyl)-4-[4-fluoro-3-(trifluoromethyl)phenyl]-1H-pyrazole (CCD ID: 4OE) (formula: C₁₆H₉F₅N₂).



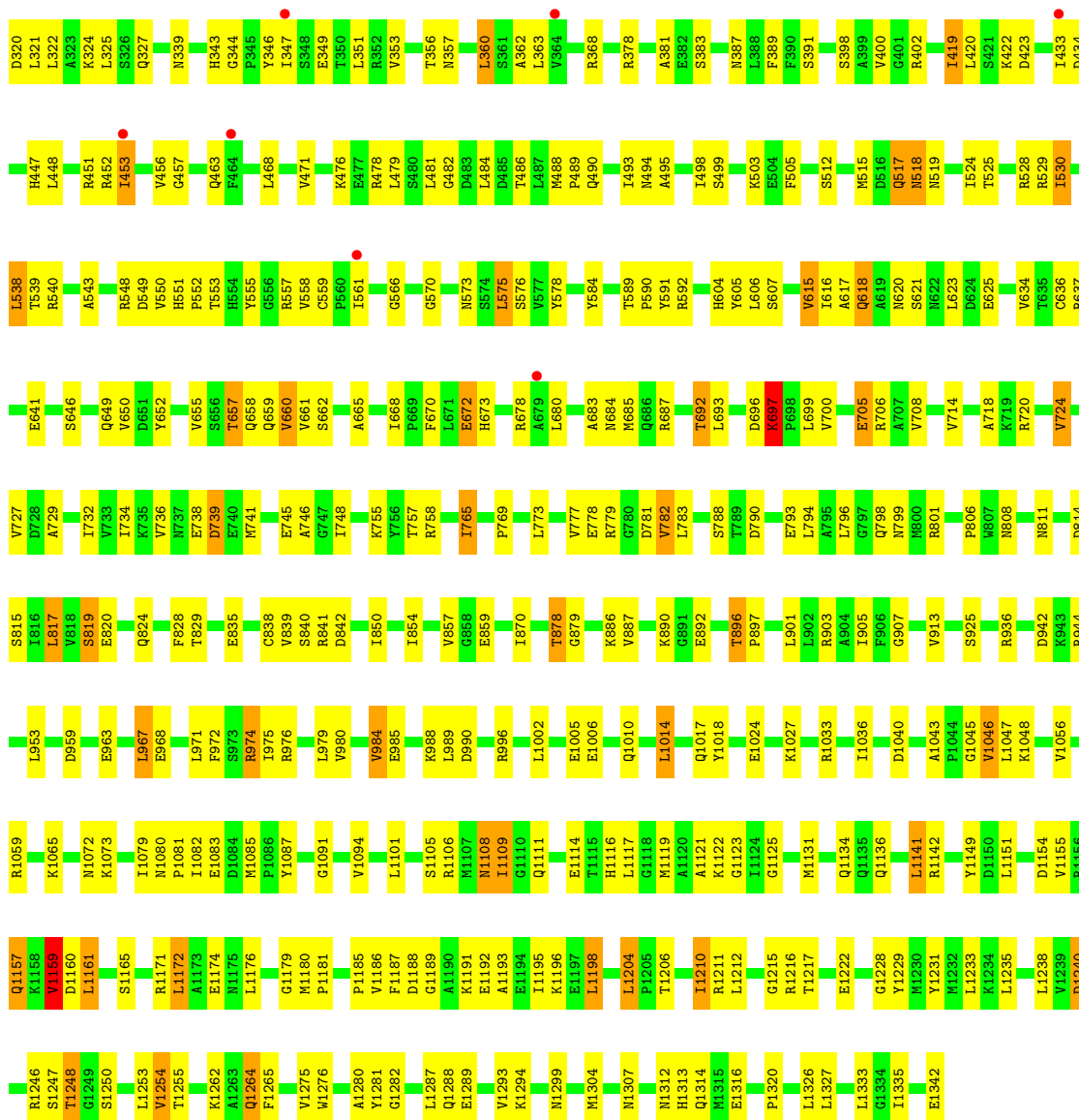
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	F	N	0	0
			23	16	5	2		
6	I	1	Total	C	F	N	0	0
			23	16	5	2		

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

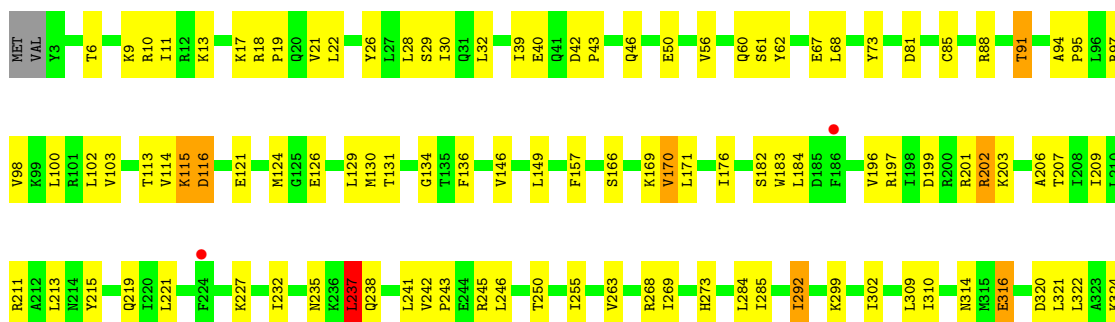
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	Mg	0	0
			1	1		
7	J	1	Total	Mg	0	0
			1	1		

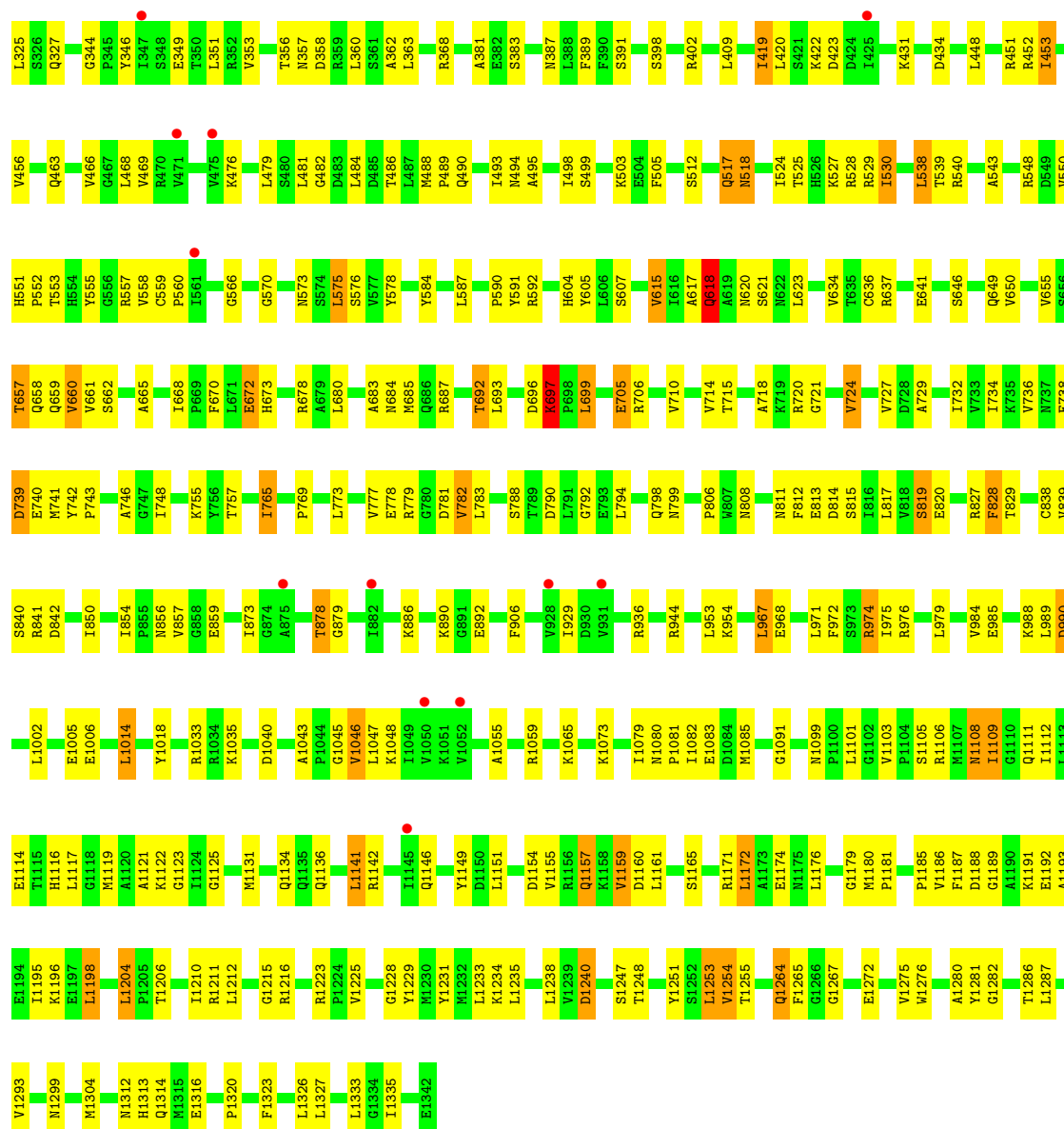
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

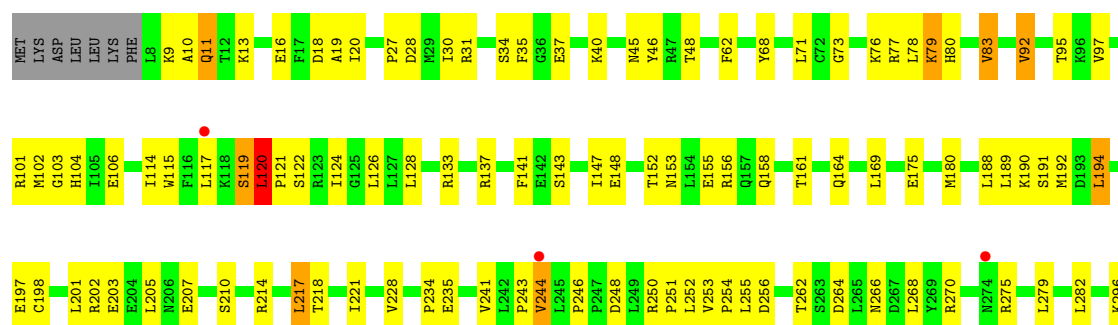


• Molecule 2: DNA-directed RNA polymerase subunit beta





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

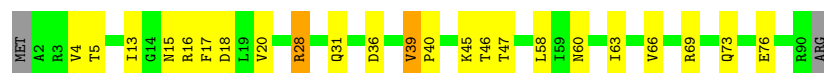






- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 73% 23% .

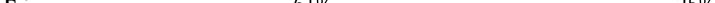


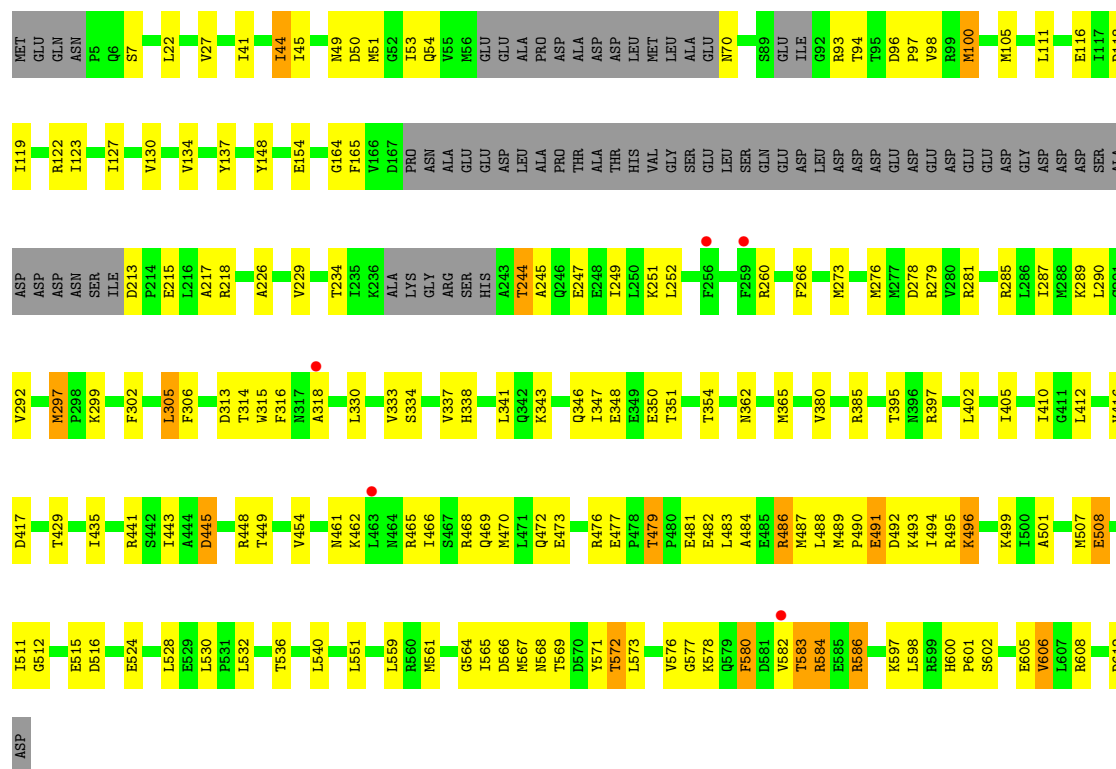
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 59% 23% 0 13%

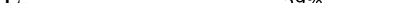


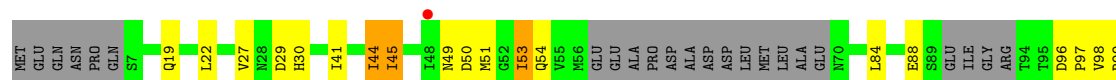
- Molecule 5: RNA polymerase sigma factor RpoD

Chain F:  61% 25% 12%



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L:  59% 26% • 12%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.58Å 204.10Å 308.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.99 49.20 – 3.99	Depositor EDS
% Data completeness (in resolution range)	93.1 (49.20-3.99) 92.2 (49.20-3.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.250 , 0.283 0.249 , 0.280	Depositor DCC
R_{free} test set	1978 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	156.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 169.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	57539	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 4OE, MG

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	0.49	1/2358 (0.0%)	0.96	2/3197 (0.1%)
1	B	0.55	0/1687	1.17	11/2286 (0.5%)
1	G	0.46	0/1751	1.00	2/2373 (0.1%)
1	H	0.49	0/1681	1.08	9/2278 (0.4%)
2	C	0.37	0/10739	0.80	13/14489 (0.1%)
2	I	0.35	1/10735 (0.0%)	0.80	13/14484 (0.1%)
3	D	0.38	0/9130	0.84	13/12325 (0.1%)
3	J	0.36	0/10409	0.83	13/14059 (0.1%)
4	E	0.40	0/693	0.84	0/935
4	K	0.36	0/629	0.84	0/847
5	F	0.39	0/4254	0.84	4/5731 (0.1%)
5	L	0.38	0/4246	0.83	9/5720 (0.2%)
All	All	0.39	2/58312 (0.0%)	0.85	89/78724 (0.1%)

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
3	D	0	1
3	J	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	954	LYS	CD-CE	-6.23	1.33	1.52
1	A	317	ARG	CD-NE	5.06	1.53	1.46

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	29	GLU	CA-C-N	-16.60	104.05	120.31
1	B	29	GLU	C-N-CA	-16.60	104.05	120.31
3	J	120	LEU	CA-C-N	-11.39	105.60	119.84
3	J	120	LEU	C-N-CA	-11.39	105.60	119.84
1	H	29	GLU	CA-C-N	-10.00	107.35	119.84
1	H	29	GLU	C-N-CA	-10.00	107.35	119.84
3	D	120	LEU	CA-C-N	-9.75	107.66	119.84
3	D	120	LEU	C-N-CA	-9.75	107.66	119.84
3	D	120	LEU	N-CA-C	7.69	126.80	109.81
3	J	120	LEU	N-CA-C	7.17	125.66	109.81
1	B	41	ASN	N-CA-C	6.87	118.56	111.14
3	J	40	LYS	CA-C-N	6.64	126.78	119.87
3	J	40	LYS	C-N-CA	6.64	126.78	119.87
2	I	1316	GLU	CA-C-N	6.58	125.82	118.97
2	I	1316	GLU	C-N-CA	6.58	125.82	118.97
1	B	150	ARG	N-CA-C	-6.52	104.64	112.59
2	I	1157	GLN	N-CA-C	6.36	118.77	111.02
2	I	954	LYS	CB-CA-C	-6.35	100.82	110.92
2	C	1157	GLN	N-CA-C	6.30	118.70	111.02
5	L	584	ARG	N-CA-C	6.27	117.28	108.00
2	I	482	GLY	N-CA-C	6.24	118.66	111.36
1	H	108	GLY	CA-C-N	6.21	126.17	119.78
1	H	108	GLY	C-N-CA	6.21	126.17	119.78
5	F	51	MET	N-CA-C	6.19	120.14	112.59
1	B	108	GLY	CA-C-N	6.15	126.11	119.78
1	B	108	GLY	C-N-CA	6.15	126.11	119.78
3	J	757	THR	CA-C-N	6.07	126.90	120.11
3	J	757	THR	C-N-CA	6.07	126.90	120.11
5	L	51	MET	N-CA-C	6.05	119.98	112.59
1	B	153	VAL	N-CA-C	6.01	114.10	108.15
2	C	1159	VAL	N-CA-C	5.85	121.50	109.34
2	I	1159	VAL	N-CA-C	5.84	121.50	109.34
2	C	1316	GLU	CA-C-N	5.79	124.99	118.97
2	C	1316	GLU	C-N-CA	5.79	124.99	118.97
2	I	237	LEU	N-CA-C	5.72	122.99	110.80
1	H	20	SER	CB-CA-C	-5.69	110.03	116.63
2	C	237	LEU	N-CA-C	5.66	122.86	110.80
1	H	153	VAL	N-CA-C	5.62	113.71	108.15
2	I	398	SER	CB-CA-C	-5.60	109.12	115.79
1	B	144	ILE	N-CA-C	5.54	115.83	107.80
3	D	40	LYS	CA-C-N	5.54	125.63	119.87
3	D	40	LYS	C-N-CA	5.54	125.63	119.87
3	J	1293	GLU	CB-CA-C	-5.53	109.21	115.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1210	ILE	N-CA-C	-5.53	107.36	112.83
1	B	20	SER	CB-CA-C	-5.52	110.23	116.63
5	F	584	ARG	N-CA-C	5.51	116.15	108.00
1	B	181	GLU	N-CA-C	-5.48	105.39	112.68
2	C	398	SER	CB-CA-C	-5.46	109.30	115.79
1	H	178	SER	CA-C-N	5.46	125.12	119.56
1	H	178	SER	C-N-CA	5.46	125.12	119.56
1	H	144	ILE	N-CA-C	5.44	115.69	107.80
3	D	1225	GLY	N-CA-C	5.41	118.29	111.09
3	J	19	ALA	CB-CA-C	-5.39	109.37	115.79
3	D	250	ARG	CA-C-N	5.36	125.30	119.78
3	D	250	ARG	C-N-CA	5.36	125.30	119.78
1	G	180	VAL	N-CA-C	5.33	115.92	108.89
2	I	566	GLY	CA-C-N	5.30	125.37	119.32
2	I	566	GLY	C-N-CA	5.30	125.37	119.32
3	J	246	PRO	CA-C-N	5.29	124.92	119.05
3	J	246	PRO	C-N-CA	5.29	124.92	119.05
2	C	566	GLY	CA-C-N	5.26	125.31	119.32
2	C	566	GLY	C-N-CA	5.26	125.31	119.32
1	G	159	ILE	N-CA-C	5.25	114.86	106.88
2	I	573	ASN	CB-CA-C	-5.25	108.96	115.89
5	L	584	ARG	CB-CA-C	-5.22	109.03	116.34
3	D	757	THR	CA-C-N	5.20	125.93	120.11
3	D	757	THR	C-N-CA	5.20	125.93	120.11
2	C	896	THR	CA-C-N	5.18	124.63	119.24
2	C	896	THR	C-N-CA	5.18	124.63	119.24
3	J	752	GLY	N-CA-C	-5.15	108.56	114.69
2	C	573	ASN	CB-CA-C	-5.14	109.11	115.89
5	L	96	ASP	CA-C-N	5.13	126.25	119.84
5	L	96	ASP	C-N-CA	5.13	126.25	119.84
3	D	501	VAL	CA-C-N	5.12	125.12	119.90
3	D	501	VAL	C-N-CA	5.12	125.12	119.90
1	B	29	GLU	C-N-CD	5.11	145.96	125.00
2	I	618	GLN	N-CA-C	5.11	118.07	109.95
2	I	1264	GLN	N-CA-C	-5.10	102.09	109.59
1	A	287	VAL	CB-CA-C	-5.10	105.18	111.70
5	L	53	ILE	N-CA-C	5.09	119.93	109.34
3	J	1210	ILE	N-CA-C	-5.07	107.81	112.83
2	C	625	GLU	CB-CA-C	-5.06	110.35	117.23
2	C	199	ASP	CB-CA-C	-5.06	109.26	116.34
5	L	84	LEU	N-CA-C	-5.05	105.96	111.82
1	A	134	THR	N-CA-C	5.04	119.48	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	213	ASP	CA-C-N	5.04	124.64	119.05
5	F	213	ASP	C-N-CA	5.04	124.64	119.05
5	L	213	ASP	CA-C-N	5.02	124.62	119.05
5	L	213	ASP	C-N-CA	5.02	124.62	119.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	120	LEU	Peptide
3	J	120	LEU	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	2328	0	2380	75	0
1	B	1667	0	1692	64	0
1	G	1730	0	1756	73	0
1	H	1662	0	1687	67	0
2	C	10570	0	10582	290	0
2	I	10566	0	10576	273	0
3	D	8992	0	9180	284	0
3	J	10254	0	10461	325	0
4	E	691	0	695	14	0
4	K	627	0	634	19	0
5	F	4204	0	4106	105	0
5	L	4196	0	4103	115	0
6	C	23	0	9	5	0
6	I	23	0	9	4	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
All	All	57539	0	57870	1530	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 13.

All (1530) 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	1.41	1.01
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.46	0.97
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.48	0.95
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.39	0.88
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.56	0.87
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.58	0.86
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.58	0.85
3:D:418:GLU:HG3	4:E:45:LYS:H	1.42	0.85
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.58	0.84
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.83
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.61	0.83
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.61	0.83
1:H:28:LEU:HB3	1:H:31:LEU:HD21	1.61	0.82
3:D:755:ILE:HD13	3:D:774:ILE:HD11	1.59	0.82
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.63	0.81
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.61	0.80
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.45	0.80
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.62	0.79
3:J:418:GLU:HG3	4:K:45:LYS:H	1.46	0.79
1:A:231:PHE:HE2	1:B:43:LEU:HD21	1.46	0.79
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.65	0.79
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.78
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.64	0.78
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.65	0.78
3:D:392:THR:HG21	5:F:606:VAL:HA	1.64	0.78
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.64	0.77
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.66	0.77
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.67	0.77
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.68	0.76
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.67	0.75
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.34	0.75
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.68	0.75
3:J:755:ILE:HD13	3:J:774:ILE:HD11	1.69	0.74
3:J:755:ILE:HG22	3:J:757:THR:H	1.51	0.74
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.69	0.74
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.69	0.74
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.52	0.73
1:H:101:THR:HG22	1:H:116:THR:HB	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.70	0.73
1:H:59:VAL:O	1:H:171:LEU:N	2.22	0.73
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.71	0.73
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.71	0.73
1:B:101:THR:HG22	1:B:116:THR:HB	1.71	0.73
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.69	0.73
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.70	0.72
5:F:561:MET:HA	5:F:567:MET:HE1	1.71	0.72
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.54	0.72
6:I:2001:4OE:H9	3:J:774:ILE:HB	1.71	0.72
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.36	0.72
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.23	0.72
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.72	0.72
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.70	0.72
1:G:23:HIS:HB2	1:G:205:MET:O	1.90	0.71
1:A:23:HIS:HB2	1:A:205:MET:O	1.90	0.71
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.72	0.71
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.72	0.71
2:C:18:ARG:NH2	2:C:620:ASN:OD1	2.23	0.71
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.24	0.71
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.72	0.71
1:H:29:GLU:HB3	1:H:30:PRO:CD	2.20	0.71
2:I:203:LYS:HB2	5:L:29:ASP:HB2	1.72	0.71
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.71	0.70
2:I:452:ARG:NH1	2:I:584:TYR:O	2.24	0.70
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.72	0.70
5:L:561:MET:HA	5:L:567:MET:HE1	1.72	0.70
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.23	0.70
5:L:470:MET:HA	5:L:473:GLU:HB3	1.73	0.70
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.72	0.70
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.23	0.70
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.54	0.70
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.56	0.70
3:D:514:THR:HG23	3:D:576:ARG:HG2	1.74	0.70
2:I:528:ARG:NH2	2:I:576:SER:O	2.24	0.70
3:D:120:LEU:HD22	3:D:121:PRO:HD3	1.73	0.69
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.73	0.69
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.75	0.69
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.74	0.69
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.22	0.69
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.74	0.69
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.40	0.68
3:D:133:ARG:NH2	5:F:93:ARG:O	2.25	0.68
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.74	0.68
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.75	0.68
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.59	0.68
2:I:18:ARG:NH1	2:I:621:SER:O	2.27	0.67
2:I:18:ARG:NH2	2:I:620:ASN:OD1	2.27	0.67
5:F:602:SER:H	5:F:605:GLU:HG3	1.59	0.67
5:F:470:MET:HA	5:F:473:GLU:HB3	1.74	0.67
1:A:166:ARG:O	1:A:168:ILE:N	2.27	0.67
2:C:452:ARG:NH1	2:C:584:TYR:O	2.28	0.67
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.75	0.67
1:H:191:ARG:NH2	3:J:410:ASP:OD2	2.27	0.67
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.28	0.67
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.77	0.67
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.75	0.67
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.60	0.67
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.76	0.66
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.78	0.66
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.76	0.66
2:I:808:ASN:H	3:J:633:ALA:HB2	1.60	0.66
3:D:356:THR:OG1	3:D:357:VAL:N	2.29	0.66
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.44	0.66
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.77	0.66
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.77	0.66
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.76	0.66
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.78	0.66
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.78	0.66
2:C:18:ARG:NH1	2:C:621:SER:O	2.29	0.65
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.78	0.65
1:G:39:LEU:HD11	1:H:227:GLN:HB3	1.77	0.65
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.61	0.65
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.78	0.65
1:A:61:ILE:HG22	1:A:62:ASP:H	1.61	0.65
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.78	0.65
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.65
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.77	0.65
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.77	0.65
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:755:ILE:HG22	3:D:757:THR:H	1.60	0.64
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.78	0.64
1:A:231:PHE:HE2	1:B:43:LEU:CD2	2.10	0.64
2:I:88:ARG:NH2	2:I:1035:LYS:O	2.30	0.64
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.60	0.64
5:F:602:SER:H	5:F:605:GLU:CD	2.05	0.64
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.79	0.64
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.80	0.64
2:I:197:ARG:HH12	5:L:29:ASP:HB3	1.62	0.64
2:I:829:THR:HA	2:I:1059:ARG:HA	1.80	0.64
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.80	0.64
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.80	0.64
3:J:748:ALA:O	3:J:777:HIS:HD2	1.80	0.64
1:G:61:ILE:HG22	1:G:62:ASP:H	1.62	0.64
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.80	0.64
5:F:461:ASN:O	5:F:465:ARG:HG2	1.98	0.64
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.79	0.64
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.80	0.63
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.80	0.63
5:L:593:LYS:HE2	5:L:596:ARG:HD3	1.79	0.63
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.63	0.63
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.63	0.63
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.81	0.63
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.80	0.63
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.79	0.63
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.81	0.63
3:D:77:ARG:HE	5:F:569:THR:HA	1.64	0.63
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.31	0.63
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.81	0.62
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.81	0.62
1:B:51:MET:HB3	1:B:178:SER:HA	1.81	0.62
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.80	0.62
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.80	0.62
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.82	0.62
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.82	0.62
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.32	0.62
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.81	0.62
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.82	0.62
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.82	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.82	0.62
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.81	0.61
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.82	0.61
1:H:29:GLU:CB	1:H:30:PRO:HD3	2.25	0.61
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.81	0.61
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.81	0.61
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.65	0.61
5:F:276:MET:SD	5:F:279:ARG:NH1	2.74	0.61
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.81	0.61
2:I:1151:LEU:HD21	2:I:1198:LEU:HD23	1.82	0.61
6:C:2001:4OE:H8	3:D:773:PHE:HB3	1.83	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.64	0.61
3:D:709:ARG:C	3:D:711:GLY:H	2.08	0.61
1:H:14:VAL:HG11	1:H:29:GLU:HG2	1.83	0.61
2:I:207:THR:HG21	2:I:351:LEU:HG	1.82	0.61
5:L:225:ARG:O	5:L:229:VAL:HG13	2.00	0.61
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.82	0.61
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.82	0.61
3:D:749:LYS:HG3	3:D:751:ASP:HB3	1.82	0.61
1:A:231:PHE:CE2	1:B:43:LEU:HD21	2.32	0.61
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.17	0.61
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.34	0.61
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.83	0.60
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.83	0.60
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.83	0.60
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.81	0.60
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.83	0.60
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.82	0.60
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.84	0.60
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.84	0.60
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.64	0.60
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.83	0.60
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.14	0.60
5:F:49:ASN:HA	5:F:53:ILE:HA	1.83	0.60
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.84	0.60
1:A:250:ASP:HB2	5:F:605:GLU:HG2	1.83	0.60
2:I:738:GLU:HA	2:I:741:MET:HE2	1.84	0.60
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.34	0.60
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.84	0.60
5:F:602:SER:H	5:F:605:GLU:CG	2.15	0.60
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.35	0.60
6:C:2001:4OE:H9	3:D:774:ILE:HB	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.66	0.60
1:G:12:ARG:HG2	1:G:13:LEU:H	1.66	0.60
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.35	0.59
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.84	0.59
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.82	0.59
3:D:741:ALA:O	3:D:762:ASN:ND2	2.35	0.59
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.84	0.59
3:J:148:GLU:H	3:J:156:ARG:HG3	1.66	0.59
3:J:356:THR:OG1	3:J:357:VAL:N	2.32	0.59
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.19	0.59
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.84	0.59
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.84	0.59
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.84	0.59
3:D:1310:THR:HG21	5:F:70:ASN:HA	1.85	0.59
3:J:308:ASP:OD2	3:J:311:ARG:NH2	2.34	0.59
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.85	0.59
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.84	0.59
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.67	0.59
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.83	0.59
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.84	0.59
2:C:136:PHE:O	2:C:143:ARG:N	2.29	0.59
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.84	0.59
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.85	0.59
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.84	0.59
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.68	0.59
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.83	0.59
1:A:45:ARG:HG2	1:B:38:THR:HB	1.85	0.59
6:I:2001:4OE:H8	3:J:773:PHE:HB3	1.85	0.59
2:C:40:GLU:O	2:C:73:TYR:OH	2.20	0.58
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.85	0.58
3:D:115:TRP:O	3:D:119:SER:HB2	2.03	0.58
3:J:210:SER:O	3:J:214:ARG:HG2	2.03	0.58
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.67	0.58
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.84	0.58
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.84	0.58
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.86	0.58
1:B:61:ILE:HB	1:B:64:VAL:O	2.03	0.58
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.85	0.58
5:F:111:LEU:HD13	5:F:116:GLU:HG2	1.85	0.58
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.84	0.58
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:829:THR:HA	2:C:1059:ARG:HA	1.84	0.58
3:D:708:ASN:HB3	3:D:712:GLN:O	2.03	0.58
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.84	0.58
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.84	0.58
5:L:111:LEU:HD13	5:L:116:GLU:HG2	1.85	0.58
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.85	0.58
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.85	0.58
1:A:12:ARG:HG2	1:A:13:LEU:H	1.69	0.58
1:A:310:ARG:O	5:F:608:ARG:NH1	2.37	0.58
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.84	0.58
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.85	0.58
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.85	0.58
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.86	0.58
1:G:12:ARG:H	1:G:30:PRO:HD2	1.67	0.58
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.37	0.58
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.84	0.58
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.67	0.58
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.86	0.58
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.86	0.58
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.86	0.58
5:L:476:ARG:HG2	5:L:477:GLU:HG2	1.85	0.58
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.86	0.58
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.86	0.58
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.36	0.58
5:L:134:VAL:HA	5:L:273:MET:HE1	1.85	0.58
2:C:30:ILE:HD12	2:C:30:ILE:H	1.68	0.57
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.85	0.57
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.70	0.57
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.86	0.57
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.87	0.57
2:C:739:ASP:OD1	2:C:739:ASP:N	2.36	0.57
3:D:1297:LYS:HB3	3:J:1303:SER:HA	1.87	0.57
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.85	0.57
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.17	0.57
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.86	0.57
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.85	0.57
2:I:30:ILE:HD12	2:I:30:ILE:H	1.69	0.57
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.68	0.57
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.40	0.57
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.85	0.57
3:D:282:LEU:HD21	5:F:410:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.86	0.57
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.86	0.57
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.86	0.57
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.87	0.57
5:L:515:GLU:HG2	5:L:516:ASP:H	1.69	0.57
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.87	0.57
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.69	0.57
2:I:494:ASN:OD1	2:I:495:ALA:N	2.36	0.57
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.85	0.57
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.87	0.57
6:I:2001:4OE:NAN	3:J:755:ILE:HG12	2.19	0.57
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.86	0.57
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.86	0.57
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.87	0.57
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.87	0.56
2:C:494:ASN:OD1	2:C:495:ALA:N	2.36	0.56
1:G:11:PRO:HD2	1:H:227:GLN:HA	1.86	0.56
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.87	0.56
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.87	0.56
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.87	0.56
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.86	0.56
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.71	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.41	0.56
2:C:1293:VAL:HG11	2:C:1304:MET:HE2	1.88	0.56
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.37	0.56
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.86	0.56
2:I:40:GLU:O	2:I:73:TYR:OH	2.23	0.56
2:I:518:ASN:OD1	2:I:518:ASN:N	2.36	0.56
5:L:49:ASN:HA	5:L:53:ILE:HA	1.87	0.56
2:C:324:LYS:O	2:C:327:GLN:NE2	2.38	0.56
3:D:847:ASP:OD1	3:D:847:ASP:N	2.38	0.56
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.38	0.56
5:F:515:GLU:HG2	5:F:516:ASP:H	1.71	0.56
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.87	0.56
2:C:1151:LEU:HD21	2:C:1198:LEU:HD23	1.87	0.56
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.69	0.56
5:L:585:GLU:O	5:L:589:GLN:HG3	2.05	0.56
1:G:228:LEU:HD11	1:H:221:ALA:HB1	1.87	0.56
1:A:14:VAL:HG22	1:A:15:ASP:H	1.71	0.56
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.88	0.56
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.88	0.56
3:D:682:VAL:O	3:D:685:ILE:HG12	2.05	0.56
5:F:476:ARG:HG2	5:F:477:GLU:HG2	1.88	0.56
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.88	0.56
5:L:551:LEU:HD22	5:L:597:LYS:HD2	1.88	0.56
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.88	0.56
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.88	0.56
5:F:483:LEU:HD12	5:F:483:LEU:H	1.70	0.56
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.38	0.56
5:L:244:THR:O	5:L:247:GLU:HG2	2.05	0.56
3:D:210:SER:O	3:D:214:ARG:HG2	2.06	0.55
2:C:488:MET:O	2:C:490:GLN:N	2.34	0.55
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.71	0.55
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.88	0.55
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.88	0.55
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.88	0.55
3:J:478:LEU:HG	4:K:47:THR:HG23	1.88	0.55
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.89	0.55
2:I:448:LEU:HB2	2:I:553:THR:HB	1.88	0.55
3:J:847:ASP:OD1	3:J:847:ASP:N	2.36	0.55
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.88	0.55
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.87	0.55
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.72	0.55
2:I:560:PRO:O	3:J:780:ARG:NH2	2.33	0.55
3:J:120:LEU:HD22	3:J:121:PRO:HD3	1.88	0.55
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.88	0.55
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.89	0.55
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.88	0.55
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.89	0.55
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.89	0.55
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.71	0.55
5:L:482:GLU:O	5:L:486:ARG:NH2	2.39	0.55
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.89	0.55
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.54
3:J:115:TRP:O	3:J:119:SER:HB2	2.07	0.54
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.72	0.54
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.90	0.54
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.89	0.54
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.89	0.54
5:F:479:THR:HG23	5:F:481:GLU:H	1.72	0.54
2:I:1320:PRO:HG2	3:J:1354:GLY:HA3	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.90	0.54
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.88	0.54
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.88	0.54
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.42	0.54
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.72	0.54
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.89	0.54
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.41	0.54
3:J:697:MET:HE1	3:J:737:ILE:HG22	1.89	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.88	0.54
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.41	0.54
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.41	0.54
5:F:482:GLU:O	5:F:486:ARG:NH2	2.41	0.54
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.90	0.54
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.40	0.54
1:A:285:THR:HG23	1:A:288:GLU:H	1.73	0.54
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.40	0.54
3:D:102:MET:HE3	3:D:246:PRO:HD3	1.89	0.54
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.23	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.89	0.54
2:C:617:ALA:HA	2:C:636:CYS:SG	2.48	0.54
5:L:602:SER:H	5:L:605:GLU:HG3	1.73	0.54
5:F:511:ILE:HG13	5:F:512:GLY:H	1.73	0.54
1:G:14:VAL:HG22	1:G:15:ASP:H	1.73	0.54
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.90	0.54
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.72	0.54
1:H:61:ILE:HB	1:H:64:VAL:O	2.08	0.54
2:I:166:SER:OG	5:L:19:GLN:O	2.20	0.54
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.90	0.54
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.90	0.54
3:J:45:ASN:HB3	3:J:48:THR:O	2.08	0.54
5:L:276:MET:SD	5:L:279:ARG:NH1	2.80	0.54
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.89	0.54
3:D:694:SER:OG	3:D:738:ARG:NE	2.36	0.54
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.89	0.54
1:G:230:ALA:HB1	1:H:12:ARG:HA	1.90	0.54
3:J:79:LYS:HG3	3:J:80:HIS:N	2.23	0.54
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.22	0.53
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.90	0.53
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.41	0.53
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1251:TYR:OH	3:J:348:ASP:OD2	2.18	0.53
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.91	0.53
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.90	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.42	0.53
2:C:518:ASN:OD1	2:C:518:ASN:N	2.40	0.53
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.73	0.53
3:D:152:THR:OG1	3:D:153:ASN:N	2.37	0.53
3:D:405:GLU:O	3:D:408:VAL:HG22	2.09	0.53
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.08	0.53
3:J:568:SER:OG	3:J:569:LEU:N	2.41	0.53
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.91	0.53
1:B:11:PRO:HA	1:B:30:PRO:HD2	1.90	0.53
1:B:13:LEU:HB3	1:B:29:GLU:CB	2.38	0.53
3:D:148:GLU:H	3:D:156:ARG:HG3	1.73	0.53
3:D:662:ALA:HA	3:D:665:GLN:HB3	1.90	0.53
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.90	0.53
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.89	0.53
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.91	0.53
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.44	0.53
3:J:733:SER:O	3:J:737:ILE:HG12	2.09	0.53
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.90	0.53
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.90	0.53
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.91	0.53
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.36	0.53
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.91	0.53
3:J:79:LYS:HB2	5:L:569:THR:H	1.74	0.53
3:J:133:ARG:HB2	5:L:88:GLU:HA	1.91	0.53
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.72	0.53
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.23	0.53
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.89	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.74	0.53
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.90	0.53
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.89	0.53
3:J:741:ALA:O	3:J:762:ASN:ND2	2.42	0.53
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.91	0.53
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.91	0.53
1:A:93:GLN:H	1:A:120:ASP:HB3	1.74	0.53
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.91	0.53
3:J:682:VAL:O	3:J:685:ILE:HG12	2.09	0.53
3:J:683:ILE:HD11	3:J:754:ILE:HG12	1.91	0.53
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.90	0.52
5:F:489:MET:HE2	5:F:493:LYS:HD2	1.90	0.52
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.43	0.52
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.92	0.52
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.91	0.52
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.91	0.52
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.91	0.52
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.74	0.52
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.91	0.52
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.09	0.52
3:D:425:ARG:HG2	3:D:426:ALA:H	1.74	0.52
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.90	0.52
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.24	0.52
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.91	0.52
3:J:1170:LYS:C	3:J:1172:LYS:H	2.18	0.52
1:A:12:ARG:H	1:A:30:PRO:HD2	1.73	0.52
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.91	0.52
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.74	0.52
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.91	0.52
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.91	0.52
2:C:738:GLU:HA	2:C:741:MET:HE2	1.91	0.52
3:D:709:ARG:O	3:D:711:GLY:N	2.40	0.52
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.43	0.52
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.91	0.52
5:F:281:ARG:O	5:F:285:ARG:HG3	2.10	0.52
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.90	0.52
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.44	0.52
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.90	0.52
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.90	0.52
2:C:339:ASN:HB3	2:C:343:HIS:H	1.75	0.52
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.92	0.52
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.91	0.52
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.92	0.52
3:J:251:PRO:HD2	5:L:507:MET:HE1	1.90	0.52
3:J:709:ARG:C	3:J:711:GLY:H	2.18	0.52
3:D:77:ARG:HG3	3:D:79:LYS:H	1.75	0.52
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.90	0.52
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.74	0.52
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.91	0.52
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.92	0.52
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:425:ARG:HG2	3:J:426:ALA:H	1.75	0.52
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.92	0.52
5:L:511:ILE:HG13	5:L:512:GLY:H	1.75	0.52
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.43	0.52
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.25	0.52
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.92	0.52
3:D:777:HIS:CE1	3:D:781:LYS:HB2	2.45	0.52
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.43	0.52
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.92	0.52
3:D:697:MET:SD	3:D:741:ALA:HB3	2.50	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.92	0.52
3:J:79:LYS:HB2	5:L:569:THR:N	2.25	0.52
3:J:298:MET:SD	5:L:402:LEU:HB3	2.49	0.52
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.92	0.52
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.92	0.51
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.91	0.51
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.91	0.51
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.92	0.51
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.92	0.51
3:D:388:ARG:NH1	3:D:414:GLU:OE1	2.43	0.51
3:D:478:LEU:HG	4:E:47:THR:HG23	1.91	0.51
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.26	0.51
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.92	0.51
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.45	0.51
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.92	0.51
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.10	0.51
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.91	0.51
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.92	0.51
2:I:206:ALA:O	2:I:209:ILE:HG22	2.10	0.51
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.91	0.51
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.74	0.51
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.91	0.51
3:J:748:ALA:HA	3:J:755:ILE:HD12	1.91	0.51
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.41	0.51
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.51
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.91	0.51
5:F:532:LEU:O	5:F:536:THR:HG23	2.11	0.51
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.91	0.51
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.93	0.51
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.45	0.51
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:613:GLY:O	3:D:617:THR:OG1	2.27	0.51
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.93	0.51
5:L:479:THR:HG23	5:L:481:GLU:H	1.76	0.51
1:A:182:ARG:C	1:A:183:ILE:HD12	2.35	0.51
2:C:9:LYS:HA	2:C:1171:ARG:HD2	1.92	0.51
2:C:641:GLU:OE2	3:D:749:LYS:NZ	2.42	0.51
2:I:237:LEU:HD22	2:I:237:LEU:H	1.75	0.51
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.91	0.51
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.91	0.51
2:C:103:VAL:HB	2:C:113:THR:HG21	1.92	0.51
3:D:189:LEU:HD22	3:D:234:PRO:HB3	1.92	0.51
5:F:487:MET:HE2	5:F:487:MET:HA	1.93	0.51
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.74	0.51
3:J:794:GLY:O	3:J:797:THR:OG1	2.24	0.51
5:L:97:PRO:HA	5:L:100:MET:HG3	1.92	0.51
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.93	0.51
1:B:91:ARG:HG2	1:B:122:GLU:O	2.11	0.51
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.76	0.51
3:D:298:MET:SD	5:F:402:LEU:HB3	2.51	0.51
1:H:29:GLU:OE2	1:H:200:LYS:HE3	2.11	0.51
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.92	0.51
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.92	0.51
2:I:1119:MET:HE3	2:I:1204:LEU:HD13	1.93	0.51
5:L:448:ARG:NH1	5:L:501:ALA:O	2.36	0.51
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.93	0.50
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.93	0.50
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.93	0.50
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.43	0.50
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.93	0.50
2:I:349:GLU:O	2:I:353:VAL:HG23	2.11	0.50
5:L:41:ILE:HA	5:L:44:ILE:HG23	1.93	0.50
5:L:483:LEU:HD12	5:L:483:LEU:H	1.75	0.50
1:B:64:VAL:HG11	1:B:69:SER:OG	2.11	0.50
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.76	0.50
3:D:712:GLN:N	3:D:712:GLN:CD	2.69	0.50
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.46	0.50
2:C:692:THR:OG1	2:C:693:LEU:N	2.43	0.50
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.93	0.50
1:G:177:TYR:O	1:G:178:SER:HB2	2.10	0.50
2:I:878:THR:OG1	2:I:879:GLY:N	2.44	0.50
2:C:557:ARG:HH21	2:C:607:SER:C	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:872:LEU:O	3:D:877:VAL:HG12	2.11	0.50
2:I:227:LYS:O	2:I:245:ARG:NH2	2.44	0.50
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.93	0.50
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.47	0.50
1:B:154:PRO:HG3	3:D:541:LEU:HD13	1.93	0.50
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.58	0.50
1:H:101:THR:H	1:H:116:THR:HG22	1.77	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.94	0.50
4:K:4:VAL:HG22	4:K:5:THR:HG23	1.94	0.50
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.94	0.50
1:G:182:ARG:O	1:G:206:GLU:N	2.45	0.50
1:G:230:ALA:CB	1:H:12:ARG:HA	2.42	0.50
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.50
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.46	0.50
2:C:402:ARG:NH2	2:C:419:ILE:O	2.45	0.50
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.77	0.50
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.93	0.50
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.93	0.50
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.92	0.50
5:F:137:TYR:HD2	5:F:273:MET:HE2	1.76	0.50
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.93	0.50
2:I:488:MET:O	2:I:490:GLN:N	2.39	0.50
3:J:1167:LYS:HE3	3:J:1168:GLU:H	1.76	0.50
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.11	0.50
5:L:582:VAL:HG22	5:L:586:ARG:HG2	1.94	0.50
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.26	0.50
1:B:151:GLY:O	1:B:177:TYR:HB2	2.12	0.50
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.94	0.50
1:G:228:LEU:CD1	1:H:221:ALA:HB1	2.42	0.50
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.94	0.50
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.77	0.50
5:L:164:GLY:O	5:L:260:ARG:HB2	2.11	0.50
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.47	0.50
5:F:573:LEU:H	5:F:573:LEU:HD23	1.76	0.50
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.93	0.50
4:K:60:ASN:HD21	4:K:63:ILE:HD13	1.77	0.50
5:L:29:ASP:OD1	5:L:30:HIS:N	2.45	0.50
2:I:103:VAL:HB	2:I:113:THR:HG21	1.93	0.49
2:I:1313:HIS:ND1	4:K:31:GLN:OE1	2.45	0.49
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.76	0.49
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.93	0.49
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.52	0.49
3:D:45:ASN:HB3	3:D:48:THR:O	2.11	0.49
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.77	0.49
3:J:198:CYS:O	3:J:202:ARG:HG3	2.11	0.49
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.12	0.49
1:A:91:ARG:HD3	1:A:210:THR:O	2.12	0.49
2:C:448:LEU:HB2	2:C:553:THR:HB	1.93	0.49
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.32	0.49
2:C:1282:GLY:O	3:D:1361:THR:N	2.44	0.49
3:D:683:ILE:HD11	3:D:754:ILE:HG12	1.95	0.49
3:D:1341:ARG:HH22	3:D:1373:ARG:HH21	1.60	0.49
1:G:102:LEU:HD12	1:G:142:MET:HE3	1.94	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.13	0.49
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.93	0.49
5:L:137:TYR:HE1	5:L:351:THR:HB	1.77	0.49
5:L:569:THR:OG1	5:L:570:ASP:N	2.37	0.49
2:C:255:ILE:HB	2:C:263:VAL:HB	1.95	0.49
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.76	0.49
3:D:596:LEU:HD11	3:D:604:MET:HE1	1.93	0.49
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	1.94	0.49
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.94	0.49
1:A:287:VAL:HG12	1:A:291:LYS:HE3	1.93	0.49
2:I:517:GLN:O	2:I:517:GLN:HG2	2.12	0.49
3:J:748:ALA:O	3:J:777:HIS:CD2	2.64	0.49
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.47	0.49
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.28	0.49
1:A:41:ASN:HB2	1:A:185:TYR:OH	2.12	0.49
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.95	0.49
2:C:349:GLU:O	2:C:353:VAL:HG23	2.12	0.49
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.95	0.49
2:C:1294:LYS:HD3	3:D:472:LEU:HG	1.95	0.49
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.93	0.49
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.94	0.49
1:H:91:ARG:HG2	1:H:122:GLU:O	2.13	0.49
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.53	0.49
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.45	0.49
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.46	0.49
2:C:207:THR:HG21	2:C:351:LEU:HG	1.95	0.49
1:G:182:ARG:C	1:G:183:ILE:HD12	2.38	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.93	0.49
2:C:115:LYS:HE3	2:C:116:ASP:H	1.77	0.49
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.95	0.49
3:D:1170:LYS:C	3:D:1172:LYS:H	2.20	0.49
1:G:93:GLN:H	1:G:120:ASP:HB3	1.78	0.49
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.48	0.49
2:C:517:GLN:HG2	2:C:517:GLN:O	2.12	0.49
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.94	0.49
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.95	0.49
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.94	0.49
3:J:613:GLY:O	3:J:617:THR:OG1	2.25	0.49
2:C:901:LEU:HB2	5:F:565:ILE:HD11	1.94	0.48
1:G:228:LEU:HD13	1:G:231:PHE:HD2	1.76	0.48
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.45	0.48
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.43	0.48
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.13	0.48
5:L:482:GLU:HG2	5:L:486:ARG:HH22	1.78	0.48
3:D:568:SER:OG	3:D:569:LEU:N	2.45	0.48
3:D:712:GLN:CD	3:D:712:GLN:H	2.14	0.48
5:F:448:ARG:NH1	5:F:501:ALA:O	2.36	0.48
1:H:221:ALA:O	1:H:224:LEU:HB3	2.12	0.48
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.95	0.48
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.95	0.48
2:C:170:VAL:HG23	2:C:171:LEU:N	2.28	0.48
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.94	0.48
2:I:316:GLU:H	2:I:316:GLU:CD	2.21	0.48
2:I:324:LYS:O	2:I:327:GLN:NE2	2.46	0.48
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.53	0.48
3:J:152:THR:OG1	3:J:153:ASN:N	2.44	0.48
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.95	0.48
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.96	0.48
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.96	0.48
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.95	0.48
3:D:733:SER:O	3:D:737:ILE:HG12	2.13	0.48
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.95	0.48
2:I:202:ARG:HH22	2:I:368:ARG:HH12	1.61	0.48
3:J:405:GLU:O	3:J:408:VAL:HG22	2.12	0.48
1:B:13:LEU:HB3	1:B:29:GLU:HB3	1.95	0.48
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.29	0.48
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.96	0.48
5:F:580:PHE:C	5:F:582:VAL:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:GLU:OE1	1:H:147:GLN:HG3	2.14	0.48
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.45	0.48
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.78	0.48
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.96	0.48
3:D:218:THR:HA	3:D:221:ILE:HG22	1.95	0.48
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.94	0.48
2:I:203:LYS:CB	5:L:29:ASP:HB2	2.43	0.48
2:I:387:ASN:HA	2:I:391:SER:HB2	1.95	0.48
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.96	0.48
3:J:1341:ARG:HH22	3:J:1373:ARG:HH21	1.60	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.13	0.48
5:L:487:MET:HA	5:L:487:MET:HE2	1.96	0.48
1:A:321:TRP:HA	1:A:322:PRO:HA	1.73	0.48
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.95	0.48
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.94	0.48
3:D:1167:LYS:HE3	3:D:1168:GLU:H	1.77	0.48
1:H:108:GLY:O	1:H:133:LEU:HB2	2.14	0.48
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.95	0.48
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.96	0.48
1:H:182:ARG:NH1	3:J:581:MET:SD	2.87	0.48
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.96	0.48
2:C:878:THR:OG1	2:C:879:GLY:N	2.44	0.48
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.79	0.48
2:I:641:GLU:OE2	3:J:749:LYS:NZ	2.36	0.48
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.96	0.48
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.47	0.48
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.96	0.48
5:L:316:PHE:HZ	5:L:334:SER:HA	1.78	0.48
5:L:489:MET:HE2	5:L:493:LYS:HD2	1.94	0.48
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.96	0.48
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.96	0.48
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.61	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.96	0.48
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.94	0.48
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.94	0.48
1:H:102:LEU:HD12	1:H:142:MET:HG2	1.95	0.48
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.95	0.48
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.96	0.48
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.96	0.48
3:J:777:HIS:CE1	3:J:781:LYS:HD2	2.49	0.48
1:A:177:TYR:O	1:A:178:SER:HB2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:VAL:O	1:A:316:MET:N	2.47	0.47
1:B:182:ARG:NH1	3:D:581:MET:SD	2.87	0.47
2:C:903:ARG:O	2:C:907:GLY:N	2.46	0.47
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.96	0.47
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.96	0.47
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.48	0.47
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.13	0.47
2:I:842:ASP:N	2:I:1045:GLY:O	2.47	0.47
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.47
3:J:481:ARG:NH1	4:K:3:ARG:O	2.47	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.94	0.47
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.49	0.47
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.94	0.47
1:B:97:GLU:OE1	1:B:147:GLN:HG3	2.14	0.47
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.95	0.47
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.95	0.47
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.94	0.47
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.96	0.47
3:J:1233:ILE:HG12	3:J:1260:MET:HE1	1.96	0.47
1:A:102:LEU:HD12	1:A:142:MET:HE3	1.96	0.47
2:C:211:ARG:NH1	2:C:357:ASN:O	2.47	0.47
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.95	0.47
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.95	0.47
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.96	0.47
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.95	0.47
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.49	0.47
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.97	0.47
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.97	0.47
2:I:250:THR:HA	2:I:268:ARG:HA	1.95	0.47
2:C:250:THR:HA	2:C:268:ARG:HA	1.96	0.47
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.96	0.47
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.21	0.47
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.96	0.47
3:J:697:MET:SD	3:J:741:ALA:HB3	2.55	0.47
1:B:44:ARG:HB3	1:B:44:ARG:NH1	2.30	0.47
2:C:227:LYS:O	2:C:245:ARG:NH2	2.48	0.47
2:C:842:ASP:N	2:C:1045:GLY:O	2.48	0.47
2:C:896:THR:HB	2:C:897:PRO:HD2	1.95	0.47
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.95	0.47
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.97	0.47
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:572:THR:O	5:F:576:VAL:HG23	2.15	0.47
1:G:28:LEU:HB2	1:G:201:LEU:HB3	1.95	0.47
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.97	0.47
1:G:230:ALA:HB2	1:H:12:ARG:HG2	1.95	0.47
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.79	0.47
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.96	0.47
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.55	0.47
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.97	0.47
1:A:282:VAL:HB	1:A:316:MET:HB2	1.95	0.47
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.96	0.47
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.97	0.47
2:C:901:LEU:O	2:C:905:ILE:HG13	2.15	0.47
2:I:26:TYR:O	2:I:29:SER:HB2	2.15	0.47
2:I:617:ALA:HA	2:I:636:CYS:SG	2.54	0.47
2:I:739:ASP:OD1	2:I:739:ASP:N	2.40	0.47
2:I:746:ALA:HB3	2:I:971:LEU:HA	1.96	0.47
2:I:806:PRO:O	3:J:633:ALA:HA	2.14	0.47
2:I:1085:MET:HA	2:I:1085:MET:HE2	1.96	0.47
5:L:287:ILE:HG12	5:L:337:VAL:HG13	1.97	0.47
1:A:182:ARG:O	1:A:183:ILE:HD12	2.14	0.47
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.96	0.47
2:C:658:GLN:O	2:C:660:VAL:N	2.48	0.47
3:D:122:SER:O	3:D:126:LEU:HG	2.14	0.47
3:D:1226:VAL:HG23	3:J:1296:GLY:HA2	1.96	0.47
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.96	0.47
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.96	0.47
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.97	0.47
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.97	0.47
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.15	0.47
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.96	0.47
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.47
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.14	0.47
3:D:1297:LYS:HG2	3:J:1302:TYR:H	1.80	0.47
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.97	0.47
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.50	0.46
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.97	0.46
3:D:128:LEU:HA	3:D:192:MET:HE1	1.98	0.46
3:D:708:ASN:OD1	3:D:708:ASN:N	2.47	0.46
1:G:79:LEU:CD1	2:I:693:LEU:HD21	2.45	0.46
2:I:255:ILE:HB	2:I:263:VAL:HB	1.96	0.46
3:J:73:GLY:O	3:J:76:LYS:NZ	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.97	0.46
1:A:54:CYS:HA	1:A:148:ARG:HG3	1.97	0.46
1:B:39:LEU:O	1:B:43:LEU:HB2	2.16	0.46
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.97	0.46
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.15	0.46
1:H:64:VAL:HG12	1:H:65:LEU:H	1.80	0.46
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.97	0.46
2:C:42:ASP:C	2:C:44:GLU:H	2.22	0.46
2:C:387:ASN:HA	2:C:391:SER:HB2	1.97	0.46
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.97	0.46
2:C:820:GLU:N	2:C:1080:ASN:O	2.49	0.46
3:D:682:VAL:HA	3:D:685:ILE:CD1	2.46	0.46
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.50	0.46
2:I:13:LYS:HZ1	2:I:1151:LEU:HB2	1.80	0.46
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.96	0.46
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.96	0.46
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.96	0.46
1:A:106:GLY:HA2	1:A:136:GLU:O	2.15	0.46
1:B:108:GLY:O	1:B:133:LEU:HB2	2.15	0.46
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.98	0.46
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.97	0.46
3:D:598:LYS:HA	3:D:601:ILE:HG22	1.96	0.46
5:F:316:PHE:HZ	5:F:334:SER:HA	1.80	0.46
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.48	0.46
2:I:1313:HIS:N	4:K:31:GLN:OE1	2.49	0.46
5:L:548:LEU:HD21	5:L:559:LEU:HD23	1.98	0.46
5:L:573:LEU:HD23	5:L:573:LEU:H	1.80	0.46
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.51	0.46
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.97	0.46
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.51	0.46
3:D:654:ILE:O	3:D:658:GLU:HB2	2.15	0.46
3:D:848:VAL:HG22	3:D:858:VAL:CG2	2.45	0.46
1:G:221:ALA:HB1	1:H:228:LEU:HD13	1.98	0.46
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.78	0.46
3:J:888:CYS:SG	3:J:890:THR:HB	2.56	0.46
1:A:54:CYS:O	1:A:146:VAL:HG13	2.15	0.46
5:F:164:GLY:O	5:F:260:ARG:HB2	2.15	0.46
2:I:705:GLU:HB2	2:I:794:LEU:HB3	1.97	0.46
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.97	0.46
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.98	0.46
1:A:172:LEU:HD12	1:A:172:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.51	0.46
3:D:9:LYS:HE2	3:D:11:GLN:HA	1.98	0.46
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.98	0.46
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.97	0.46
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.96	0.46
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.97	0.46
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.81	0.46
1:B:151:GLY:O	1:B:177:TYR:HD2	1.99	0.46
2:C:1085:MET:HE2	2:C:1085:MET:HA	1.97	0.46
3:D:901:ARG:HA	3:D:908:ILE:HA	1.96	0.46
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.97	0.46
5:F:551:LEU:HD21	5:F:598:LEU:HD21	1.98	0.46
1:G:50:SER:HB3	1:G:150:ARG:HD2	1.98	0.46
2:I:197:ARG:NH2	5:L:29:ASP:OD2	2.49	0.46
5:L:137:TYR:HD2	5:L:273:MET:HE2	1.80	0.46
5:L:572:THR:O	5:L:576:VAL:HG23	2.16	0.46
3:D:482:ALA:HB3	4:E:20:VAL:HG22	1.98	0.46
5:F:41:ILE:HA	5:F:44:ILE:HG23	1.98	0.46
5:F:583:THR:HG22	5:F:584:ARG:H	1.81	0.46
3:J:735:ALA:O	3:J:738:ARG:HB3	2.15	0.46
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.81	0.46
3:J:1025:MET:SD	3:J:1124:ILE:HD12	2.56	0.46
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.51	0.46
2:C:524:ILE:HG21	2:C:708:VAL:HG13	1.98	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.97	0.46
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.80	0.46
2:I:215:TYR:HA	2:I:219:GLN:NE2	2.31	0.46
3:J:197:GLU:O	3:J:201:LEU:HG	2.16	0.46
3:J:872:LEU:O	3:J:877:VAL:HG12	2.16	0.46
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.49	0.46
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.97	0.45
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.31	0.45
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.97	0.45
2:I:820:GLU:N	2:I:1080:ASN:O	2.48	0.45
2:I:1286:THR:N	3:J:479:GLU:OE2	2.42	0.45
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.98	0.45
4:K:73:GLN:HA	4:K:76:GLU:HB3	1.98	0.45
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.97	0.45
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.99	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.16	0.45
2:C:1333:LEU:C	2:C:1335:ILE:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.98	0.45
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.17	0.45
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.98	0.45
1:G:28:LEU:HD22	1:G:201:LEU:HD23	1.99	0.45
1:G:106:GLY:HA2	1:G:136:GLU:O	2.16	0.45
2:I:854:ILE:HB	2:I:857:VAL:HG21	1.99	0.45
3:J:709:ARG:O	3:J:711:GLY:N	2.48	0.45
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.80	0.45
3:D:77:ARG:NE	5:F:569:THR:HA	2.32	0.45
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.97	0.45
2:I:680:LEU:O	2:I:684:ASN:HB2	2.16	0.45
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.45
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.98	0.45
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.99	0.45
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.81	0.45
1:A:28:LEU:HB2	1:A:201:LEU:HB3	1.99	0.45
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.97	0.45
2:I:710:VAL:HA	2:I:715:THR:HG21	1.98	0.45
3:J:128:LEU:HA	3:J:192:MET:HE1	1.99	0.45
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.98	0.45
3:J:290:ILE:H	3:J:290:ILE:HD12	1.81	0.45
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.97	0.45
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.98	0.45
5:L:130:VAL:HB	5:L:365:MET:HG3	1.97	0.45
5:L:465:ARG:HA	5:L:468:ARG:HH12	1.82	0.45
1:B:41:ASN:CG	2:C:1217:THR:HA	2.41	0.45
3:D:62:PHE:O	3:D:101:ARG:HD2	2.17	0.45
3:D:198:CYS:O	3:D:202:ARG:HG3	2.17	0.45
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.29	0.45
3:D:1227:HIS:HD2	3:J:1293:GLU:H	1.65	0.45
5:F:601:PRO:HB2	5:F:605:GLU:OE2	2.17	0.45
1:G:228:LEU:C	1:G:230:ALA:H	2.23	0.45
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.99	0.45
2:I:553:THR:O	2:I:557:ARG:HD2	2.17	0.45
3:J:122:SER:O	3:J:126:LEU:HG	2.17	0.45
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.45
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.98	0.45
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.97	0.45
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.98	0.45
2:C:840:SER:O	2:C:1047:LEU:N	2.50	0.45
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.52	0.45
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.99	0.45
5:F:134:VAL:HA	5:F:273:MET:HE1	1.97	0.45
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.99	0.45
2:I:778:GLU:O	2:I:781:ASP:HB2	2.17	0.45
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.16	0.45
5:L:461:ASN:O	5:L:465:ARG:HG2	2.16	0.45
1:A:319:GLU:O	1:A:320:ASN:HB2	2.15	0.45
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.57	0.45
1:B:64:VAL:HG12	1:B:65:LEU:H	1.81	0.45
1:B:78:ILE:O	1:B:82:LEU:HG	2.16	0.45
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.98	0.45
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.51	0.45
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.99	0.45
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.81	0.45
2:I:402:ARG:NH2	2:I:419:ILE:O	2.50	0.45
3:J:266:ASN:O	3:J:270:ARG:HB2	2.17	0.45
3:J:810:THR:HG23	3:J:811:GLU:H	1.81	0.45
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.52	0.45
1:B:182:ARG:HD2	3:D:581:MET:HE1	1.99	0.45
2:C:680:LEU:O	2:C:684:ASN:HB2	2.17	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.45
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.98	0.45
2:I:115:LYS:HE3	2:I:116:ASP:H	1.82	0.45
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.98	0.45
2:I:1282:GLY:O	3:J:1361:THR:N	2.49	0.45
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.99	0.45
3:J:901:ARG:HD2	3:J:906:GLY:O	2.16	0.45
3:J:1078:LEU:HB3	3:J:1121:LEU:HD13	1.98	0.45
5:L:580:PHE:C	5:L:582:VAL:H	2.25	0.45
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.52	0.45
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.98	0.45
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.32	0.45
1:G:58:GLU:HB2	1:G:145:LYS:HB3	1.98	0.45
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.57	0.45
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.52	0.45
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.17	0.45
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.97	0.44
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.98	0.44
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.49	0.44
3:D:251:PRO:HD2	5:F:507:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:598:LYS:O	3:D:601:ILE:HG22	2.17	0.44
5:F:346:GLN:O	5:F:350:GLU:HG3	2.17	0.44
5:F:380:VAL:HG22	5:F:416:VAL:HG21	1.98	0.44
3:J:668:PHE:HB2	3:J:678:ARG:HG3	1.99	0.44
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.81	0.44
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.17	0.44
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.49	0.44
2:C:12:ARG:HH21	2:C:793:GLU:CD	2.24	0.44
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.17	0.44
2:I:232:ILE:HG12	2:I:237:LEU:HD13	1.99	0.44
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.99	0.44
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.32	0.44
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.16	0.44
3:D:657:ALA:O	3:D:661:VAL:HG13	2.17	0.44
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.98	0.44
5:F:465:ARG:HA	5:F:468:ARG:HH12	1.83	0.44
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.99	0.44
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.81	0.44
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.98	0.44
3:J:70:CYS:SG	3:J:71:LEU:N	2.90	0.44
3:J:1244:GLN:HE21	3:J:1244:GLN:HB3	1.59	0.44
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.53	0.44
2:C:808:ASN:H	3:D:633:ALA:HB2	1.82	0.44
2:C:897:PRO:HB3	5:F:564:GLY:C	2.42	0.44
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.28	0.44
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.99	0.44
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.33	0.44
3:D:860:ARG:HB3	3:D:861:ASN:H	1.56	0.44
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.32	0.44
5:F:244:THR:O	5:F:247:GLU:HG2	2.18	0.44
2:I:828:PHE:CE2	2:I:1234:LYS:HB2	2.52	0.44
2:I:936:ARG:NH2	2:I:1043:ALA:O	2.51	0.44
2:C:124:MET:HB2	2:C:498:ILE:HD13	2.00	0.44
2:C:213:LEU:HD13	2:C:422:LYS:HG2	1.98	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.99	0.44
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.80	0.44
2:I:130:MET:SD	2:I:134:GLY:HA2	2.58	0.44
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.98	0.44
3:J:203:GLU:O	3:J:207:GLU:HG2	2.18	0.44
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.83	0.44
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.99	0.44
1:G:182:ARG:HB3	1:G:206:GLU:HB3	2.00	0.44
2:I:356:THR:HG21	2:I:362:ALA:HA	1.99	0.44
2:I:557:ARG:HH21	2:I:607:SER:C	2.25	0.44
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.98	0.44
3:J:50:LYS:HB3	3:J:71:LEU:HD21	2.00	0.44
3:J:660:GLU:O	3:J:664:ILE:HG12	2.17	0.44
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.82	0.44
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.50	0.44
3:J:506:VAL:HG23	3:J:628:GLY:HA3	2.00	0.44
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.99	0.44
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.00	0.44
3:J:708:ASN:OD1	3:J:708:ASN:N	2.49	0.44
5:L:127:ILE:O	5:L:130:VAL:HG22	2.18	0.44
2:C:237:LEU:H	2:C:237:LEU:HD22	1.82	0.44
3:D:266:ASN:O	3:D:270:ARG:HB2	2.17	0.44
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.84	0.44
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.82	0.44
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.99	0.44
3:J:598:LYS:O	3:J:601:ILE:HG22	2.18	0.44
3:J:697:MET:O	3:J:701:LEU:HB2	2.18	0.44
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.51	0.44
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.99	0.44
3:D:156:ARG:NH2	3:D:191:SER:OG	2.46	0.44
3:D:701:LEU:HD13	3:D:723:TYR:HB2	1.99	0.44
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.86	0.44
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.00	0.44
1:G:54:CYS:HA	1:G:148:ARG:HG3	1.98	0.44
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.18	0.44
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.86	0.44
1:B:221:ALA:O	1:B:224:LEU:HB3	2.18	0.43
2:C:53:PHE:O	2:C:57:PHE:HB2	2.19	0.43
2:C:499:SER:O	2:C:503:LYS:HB2	2.18	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.58	0.43
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.99	0.43
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.18	0.43
3:J:385:LEU:HD11	3:J:408:VAL:HG12	2.00	0.43
3:J:694:SER:OG	3:J:738:ARG:NE	2.42	0.43
3:J:1349:GLU:OE2	3:J:1349:GLU:N	2.38	0.43
1:B:61:ILE:HG21	1:B:78:ILE:HD13	1.99	0.43
3:D:197:GLU:O	3:D:201:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.99	0.43
2:I:814:ASP:CG	2:I:1106:ARG:HH12	2.22	0.43
1:A:79:LEU:CD1	2:C:693:LEU:HD21	2.49	0.43
1:B:57:THR:HG22	1:B:58:GLU:HG2	2.00	0.43
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.33	0.43
2:C:356:THR:HG21	2:C:362:ALA:HA	1.99	0.43
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	2.01	0.43
3:D:161:THR:HG22	3:D:164:GLN:CD	2.44	0.43
3:D:308:ASP:OD2	3:D:311:ARG:NH2	2.43	0.43
3:D:384:LYS:HD2	3:D:387:LEU:HD23	1.99	0.43
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.85	0.43
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.99	0.43
3:D:1233:ILE:HG12	3:D:1260:MET:HE1	2.00	0.43
2:I:813:GLU:HA	3:J:504:GLN:NE2	2.33	0.43
3:J:190:LYS:HD3	3:J:235:GLU:HG2	2.00	0.43
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.00	0.43
3:J:611:ILE:HG22	3:J:612:LEU:HD12	2.00	0.43
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.00	0.43
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.91	0.43
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	2.01	0.43
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.83	0.43
6:C:2001:4OE:CAL	3:D:755:ILE:HG12	2.48	0.43
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.00	0.43
3:D:777:HIS:CE1	3:D:781:LYS:HD2	2.53	0.43
5:F:462:LYS:O	5:F:466:ILE:HG13	2.17	0.43
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.54	0.43
1:H:16:ILE:HG13	1:H:26:VAL:HG22	2.00	0.43
2:I:720:ARG:HA	2:I:779:ARG:HG3	2.00	0.43
3:J:484:MET:HE2	3:J:484:MET:HB3	1.84	0.43
3:J:1048:ARG:NH2	3:J:1057:SER:HB2	2.33	0.43
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.88	0.43
2:C:360:LEU:HB2	2:C:378:ARG:HH21	1.83	0.43
3:D:426:ALA:HB3	3:D:427:PRO:HD3	2.00	0.43
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	2.00	0.43
5:F:137:TYR:HE1	5:F:351:THR:HB	1.83	0.43
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.52	0.43
3:J:422:LEU:HD13	3:J:471:PRO:HG3	2.00	0.43
3:J:1348:LYS:HD2	3:J:1348:LYS:HA	1.84	0.43
2:C:238:GLN:HB3	2:C:284:LEU:HD11	2.00	0.43
2:C:1121:ALA:HB1	2:C:1180:MET:O	2.18	0.43
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:170:VAL:HG23	2:I:171:LEU:N	2.32	0.43
3:J:34:SER:OG	3:J:104:HIS:ND1	2.30	0.43
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.83	0.43
2:C:83:GLN:O	2:C:87:ILE:HG13	2.19	0.43
2:C:724:VAL:HG11	2:C:727:VAL:HG22	2.00	0.43
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.51	0.43
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.99	0.43
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.34	0.43
3:J:969:SER:HB3	3:J:1116:SER:HB2	2.01	0.43
4:K:49:ILE:HA	4:K:52:ARG:HD3	2.01	0.43
2:C:552:PRO:HG3	6:C:2001:4OE:CAQ	2.49	0.43
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	2.00	0.43
2:C:953:LEU:HD12	2:C:1036:ILE:HD12	2.00	0.43
2:C:1247:SER:OG	2:C:1248:THR:N	2.52	0.43
3:D:264:ASP:OD2	3:D:264:ASP:N	2.52	0.43
5:F:511:ILE:HD12	5:F:511:ILE:HA	1.84	0.43
2:I:499:SER:O	2:I:503:LYS:HB2	2.18	0.43
2:I:721:GLY:N	2:I:740:GLU:OE1	2.47	0.43
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.54	0.43
5:L:561:MET:HE3	5:L:561:MET:HB2	1.91	0.43
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.82	0.43
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.01	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.01	0.43
2:I:551:HIS:ND1	2:I:552:PRO:HD2	2.34	0.43
2:I:692:THR:OG1	2:I:827:ARG:O	2.34	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.53	0.43
3:J:62:PHE:O	3:J:101:ARG:HD2	2.19	0.43
3:J:848:VAL:HG22	3:J:858:VAL:CG2	2.48	0.43
3:J:987:GLU:H	3:J:987:GLU:HG3	1.61	0.43
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.83	0.43
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.34	0.43
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.19	0.43
5:L:234:THR:O	5:L:245:ALA:HB2	2.18	0.43
1:B:100:LEU:HB2	1:B:144:ILE:HG23	2.01	0.43
2:C:316:GLU:CD	2:C:316:GLU:H	2.27	0.43
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.59	0.43
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.51	0.43
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	2.01	0.43
5:F:22:LEU:H	5:F:54:GLN:CB	2.32	0.43
5:F:582:VAL:HG22	5:F:586:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.34	0.43
2:I:68:LEU:HD11	2:I:100:LEU:HB3	2.00	0.43
3:J:274:ASN:ND2	5:L:446:GLN:HB2	2.34	0.43
3:J:479:GLU:HG3	4:K:20:VAL:HG11	2.00	0.43
1:B:16:ILE:HG13	1:B:26:VAL:HG22	2.00	0.42
1:B:101:THR:HG23	1:B:103:ASN:H	1.84	0.42
2:C:383:SER:O	2:C:387:ASN:HB2	2.19	0.42
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.47	0.42
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	2.01	0.42
5:F:469:GLN:O	5:F:472:GLN:NE2	2.53	0.42
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	2.01	0.42
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.54	0.42
2:I:299:LYS:HB2	2:I:299:LYS:HE2	1.78	0.42
2:I:538:LEU:H	2:I:538:LEU:HG	1.62	0.42
2:I:976:ARG:NH2	2:I:990:ASP:OD2	2.52	0.42
3:J:287:ALA:HB3	3:J:292:VAL:HG13	2.01	0.42
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.54	0.42
5:L:124:GLU:O	5:L:128:ASN:HB2	2.19	0.42
5:L:297:MET:HE3	5:L:330:LEU:HD11	2.01	0.42
1:A:31:LEU:HD13	1:A:36:GLY:HA2	2.00	0.42
1:A:51:MET:HE3	1:A:52:PRO:HD2	2.01	0.42
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.00	0.42
1:A:231:PHE:CE2	1:B:43:LEU:CD2	2.96	0.42
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.01	0.42
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.34	0.42
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.54	0.42
5:F:348:GLU:HG2	5:F:354:THR:HA	2.00	0.42
2:I:658:GLN:O	2:I:660:VAL:N	2.52	0.42
2:I:742:TYR:O	2:I:974:ARG:NH2	2.52	0.42
6:I:2001:4OE:CAL	3:J:755:ILE:HG12	2.49	0.42
2:C:555:TYR:C	2:C:557:ARG:H	2.26	0.42
2:C:778:GLU:O	2:C:781:ASP:HB2	2.20	0.42
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	2.02	0.42
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.54	0.42
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.17	0.42
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.84	0.42
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.34	0.42
2:I:538:LEU:HD22	2:I:543:ALA:HB2	2.00	0.42
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.84	0.42
3:J:513:MET:HE1	3:J:579:LEU:HD13	2.00	0.42
3:J:863:LEU:HD11	3:J:901:ARG:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:HA	1:B:180:VAL:HG21	2.01	0.42
2:C:548:ARG:O	2:C:570:GLY:HA3	2.19	0.42
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.00	0.42
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.49	0.42
2:C:980:VAL:HA	2:C:984:VAL:HA	2.00	0.42
1:H:64:VAL:HG21	1:H:69:SER:CB	2.48	0.42
1:H:100:LEU:HB2	1:H:144:ILE:HG23	2.01	0.42
2:I:383:SER:O	2:I:387:ASN:HB2	2.19	0.42
2:I:1121:ALA:HB1	2:I:1180:MET:O	2.20	0.42
2:I:1123:GLY:HA3	2:I:1204:LEU:HD11	2.01	0.42
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.84	0.42
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.92	0.42
5:L:348:GLU:HG2	5:L:354:THR:HA	2.02	0.42
5:L:547:VAL:HG12	5:L:598:LEU:HD22	2.01	0.42
1:B:84:ASN:O	1:B:128:HIS:HE1	2.02	0.42
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.83	0.42
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.01	0.42
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.83	0.42
2:C:814:ASP:CG	2:C:1106:ARG:HH12	2.22	0.42
2:C:959:ASP:O	2:C:963:GLU:HG2	2.19	0.42
2:C:972:PHE:CD2	2:C:975:ILE:HD12	2.55	0.42
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.85	0.42
3:D:27:PRO:O	3:D:31:ARG:HG3	2.20	0.42
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.01	0.42
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.17	0.42
1:G:12:ARG:HG2	1:G:13:LEU:N	2.34	0.42
1:G:224:LEU:HD13	1:H:228:LEU:HD11	2.00	0.42
2:I:466:VAL:O	2:I:469:VAL:HG22	2.19	0.42
3:J:572:THR:OG1	3:J:573:THR:N	2.52	0.42
5:L:412:LEU:HD13	5:L:435:ILE:HD11	2.01	0.42
5:L:511:ILE:HD12	5:L:511:ILE:HA	1.87	0.42
1:A:75:GLN:HA	2:C:729:ALA:N	2.35	0.42
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.54	0.42
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	2.00	0.42
3:D:709:ARG:C	3:D:711:GLY:N	2.76	0.42
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	2.02	0.42
5:F:148:TYR:OH	5:F:218:ARG:HA	2.20	0.42
2:I:559:CYS:HA	2:I:560:PRO:HD3	1.87	0.42
2:I:1146:GLN:NE2	2:I:1160:ASP:OD1	2.52	0.42
3:J:1034:PHE:HA	3:J:1114:GLN:HA	2.02	0.42
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:51:LEU:HD23	4:K:51:LEU:HA	1.93	0.42
5:L:130:VAL:O	5:L:134:VAL:HG23	2.20	0.42
1:A:39:LEU:HD11	1:B:227:GLN:HB3	2.00	0.42
3:D:106:GLU:OE2	3:D:241:VAL:HG22	2.19	0.42
3:D:695:LYS:HD3	3:D:695:LYS:HA	1.69	0.42
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.00	0.42
3:D:919:ALA:O	3:D:923:ILE:HG13	2.20	0.42
5:F:249:ILE:O	5:F:252:LEU:HB3	2.19	0.42
1:G:54:CYS:O	1:G:146:VAL:HG13	2.19	0.42
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.17	0.42
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.54	0.42
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.20	0.42
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.27	0.42
5:L:22:LEU:H	5:L:54:GLN:CB	2.32	0.42
1:B:102:LEU:HD23	1:B:115:ILE:HG23	2.02	0.42
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.60	0.42
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.01	0.42
3:D:394:ILE:CG2	5:F:536:THR:HA	2.50	0.42
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.02	0.42
3:D:557:LYS:HA	3:D:563:LEU:HA	2.02	0.42
3:D:1372:ARG:HG3	3:J:853:THR:HB	2.01	0.42
5:F:97:PRO:HA	5:F:100:MET:HG3	2.00	0.42
5:F:343:LYS:HD2	5:F:343:LYS:H	1.85	0.42
5:F:343:LYS:O	5:F:347:ILE:HG13	2.20	0.42
1:G:79:LEU:HD11	2:I:693:LEU:HD21	2.01	0.42
2:I:211:ARG:NH1	2:I:357:ASN:O	2.53	0.42
2:I:555:TYR:C	2:I:557:ARG:H	2.28	0.42
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	2.01	0.42
3:J:264:ASP:OD2	3:J:264:ASP:N	2.52	0.42
3:J:557:LYS:HA	3:J:563:LEU:HA	2.02	0.42
3:J:1270:GLY:HA3	3:J:1298:VAL:HG22	2.02	0.42
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.91	0.42
1:A:221:ALA:HB1	1:B:228:LEU:HD22	2.01	0.42
3:D:77:ARG:HD2	3:D:78:LEU:H	1.85	0.42
3:D:203:GLU:O	3:D:207:GLU:HG2	2.20	0.42
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.85	0.42
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	2.00	0.42
5:F:234:THR:O	5:F:245:ALA:HB2	2.19	0.42
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.53	0.42
1:H:34:GLY:N	1:H:199:ASP:OD2	2.51	0.42
2:I:176:ILE:HB	2:I:184:LEU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:183:TRP:HB2	2:I:199:ASP:HA	2.02	0.42
2:I:967:LEU:HD12	2:I:967:LEU:HA	1.91	0.42
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.20	0.42
3:J:466:MET:HE2	3:J:466:MET:HB3	1.98	0.42
1:A:192:VAL:O	1:A:193:GLU:C	2.62	0.42
1:A:228:LEU:CD1	1:B:221:ALA:HB1	2.49	0.42
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.55	0.42
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.55	0.42
2:C:360:LEU:HB2	2:C:378:ARG:NH2	2.35	0.42
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.84	0.42
2:C:553:THR:O	2:C:557:ARG:HD2	2.20	0.42
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.20	0.42
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.20	0.42
3:D:1268:ASN:HB2	3:J:1268:ASN:HD22	1.85	0.42
5:F:496:LYS:HE3	5:F:496:LYS:HB2	1.88	0.42
1:H:181:GLU:HA	3:J:535:ARG:NH2	2.34	0.42
3:J:708:ASN:HB3	3:J:712:GLN:O	2.20	0.42
5:L:253:SER:O	5:L:257:LYS:HG3	2.20	0.42
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.70	0.42
1:B:50:SER:HA	1:B:151:GLY:HA2	2.01	0.41
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	2.35	0.41
3:D:73:GLY:O	3:D:76:LYS:NZ	2.38	0.41
3:D:137:ARG:HG2	3:D:143:SER:HB2	2.01	0.41
3:D:537:TYR:OH	3:D:634:ARG:NH2	2.53	0.41
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.80	0.41
3:D:870:ASP:O	3:D:874:GLU:HG2	2.20	0.41
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.84	0.41
1:G:77:ASP:O	1:G:81:ILE:HG13	2.20	0.41
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.01	0.41
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.84	0.41
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.88	0.41
2:I:724:VAL:HG11	2:I:727:VAL:HG22	2.02	0.41
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.85	0.41
3:J:843:VAL:HG11	3:J:897:HIS:O	2.20	0.41
3:J:853:THR:HG22	3:J:854:ALA:H	1.84	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.77	0.41
1:A:219:ARG:HE	1:A:219:ARG:HB2	1.74	0.41
1:B:64:VAL:HG21	1:B:69:SER:CB	2.50	0.41
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.85	0.41
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.55	0.41
5:F:380:VAL:HG13	5:F:412:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:VAL:O	1:G:193:GLU:C	2.64	0.41
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.56	0.41
1:H:182:ARG:HD2	3:J:581:MET:HE1	2.02	0.41
2:I:197:ARG:NH1	2:I:201:ARG:O	2.52	0.41
2:I:699:LEU:HD22	2:I:699:LEU:HA	1.95	0.41
3:J:137:ARG:HG2	3:J:143:SER:HB2	2.02	0.41
3:J:579:LEU:HD12	3:J:582:ILE:HD12	2.01	0.41
3:J:963:VAL:HB	3:J:980:THR:HG23	2.02	0.41
2:C:11:ILE:HD13	2:C:11:ILE:HA	1.87	0.41
2:C:498:ILE:HD12	2:C:498:ILE:H	1.85	0.41
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.85	0.41
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.20	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.93	0.41
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	2.02	0.41
5:F:297:MET:HE3	5:F:330:LEU:HD11	2.03	0.41
5:F:482:GLU:HG2	5:F:486:ARG:HH22	1.85	0.41
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.41
1:H:41:ASN:O	1:H:45:ARG:HG3	2.19	0.41
1:H:78:ILE:O	1:H:82:LEU:HG	2.21	0.41
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.02	0.41
3:J:119:SER:O	3:J:121:PRO:HD2	2.21	0.41
3:J:746:LEU:HD12	3:J:746:LEU:H	1.85	0.41
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.02	0.41
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.03	0.41
1:A:318:LEU:H	1:A:318:LEU:HD22	1.84	0.41
2:C:720:ARG:HA	2:C:779:ARG:HG3	2.01	0.41
2:C:819:SER:HB2	2:C:1085:MET:SD	2.60	0.41
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	2.02	0.41
3:D:190:LYS:HD3	3:D:235:GLU:HG2	2.02	0.41
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.50	0.41
1:G:64:VAL:HG11	1:G:78:ILE:HG21	2.02	0.41
2:I:73:TYR:HB2	2:I:98:VAL:HG22	2.02	0.41
2:I:732:ILE:HD11	2:I:769:PRO:HB3	2.02	0.41
2:I:782:VAL:HG11	2:I:792:GLY:HA2	2.03	0.41
3:J:56:LEU:HD11	3:J:273:ILE:HD12	2.02	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.02	0.41
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.55	0.41
3:J:997:VAL:HA	3:J:998:PRO:HD3	1.85	0.41
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.02	0.41
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.35	0.41
3:J:1268:ASN:OD1	3:J:1269:ALA:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:GLY:N	1:B:199:ASP:OD2	2.52	0.41
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.49	0.41
3:D:821:MET:HE3	3:D:879:ALA:HB1	2.02	0.41
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.03	0.41
1:H:109:PRO:HA	1:H:132:HIS:HA	2.02	0.41
2:I:28:LEU:HD22	2:I:527:LYS:HD2	2.02	0.41
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.94	0.41
3:J:441:LEU:HD13	3:J:441:LEU:HA	1.91	0.41
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.90	0.41
5:L:507:MET:HG2	5:L:520:GLY:HA3	2.02	0.41
1:A:102:LEU:HD22	1:A:103:ASN:H	1.86	0.41
2:C:967:LEU:HD12	2:C:967:LEU:HA	1.85	0.41
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	2.03	0.41
2:C:1161:LEU:HD12	2:C:1161:LEU:HA	1.66	0.41
3:D:202:ARG:HD3	3:J:1181:ASP:HA	2.02	0.41
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.80	0.41
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.03	0.41
3:D:735:ALA:O	3:D:738:ARG:HB3	2.20	0.41
5:F:314:THR:O	5:F:318:ALA:HB3	2.20	0.41
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	2.03	0.41
2:I:1333:LEU:C	2:I:1335:ILE:H	2.27	0.41
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.55	0.41
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.02	0.41
3:J:384:LYS:HD2	3:J:387:LEU:HD23	2.02	0.41
3:J:528:THR:HG22	3:J:532:GLU:CD	2.45	0.41
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.69	0.41
3:J:740:LEU:HD12	3:J:740:LEU:HA	1.89	0.41
3:J:800:LEU:O	3:J:803:VAL:HG12	2.20	0.41
5:L:299:LYS:O	5:L:303:ILE:HG12	2.21	0.41
5:L:401:PHE:O	5:L:405:ILE:HG23	2.21	0.41
1:A:164:ASP:C	1:A:166:ARG:H	2.28	0.41
2:C:27:LEU:HB2	2:C:524:ILE:HD11	2.02	0.41
2:C:854:ILE:HB	2:C:857:VAL:HG21	2.03	0.41
3:D:528:THR:HG22	3:D:532:GLU:CD	2.46	0.41
3:D:794:GLY:O	3:D:797:THR:OG1	2.28	0.41
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.88	0.41
1:G:75:GLN:HA	2:I:729:ALA:N	2.36	0.41
1:G:228:LEU:C	1:G:230:ALA:N	2.79	0.41
1:H:20:SER:OG	1:H:21:SER:N	2.53	0.41
2:I:62:TYR:CZ	2:I:476:LYS:HB3	2.56	0.41
2:I:91:THR:HG21	2:I:503:LYS:NZ	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:113:THR:OG1	2:I:116:ASP:OD2	2.26	0.41
2:I:1247:SER:HB3	3:J:375:GLU:O	2.21	0.41
3:J:588:PRO:O	3:J:591:ILE:HG22	2.20	0.41
5:L:41:ILE:O	5:L:45:ILE:HG22	2.21	0.41
5:L:346:GLN:O	5:L:350:GLU:HG3	2.21	0.41
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.56	0.41
1:B:20:SER:OG	1:B:21:SER:N	2.53	0.41
2:C:38:PHE:HB2	2:C:457:GLY:CA	2.50	0.41
2:C:170:VAL:HG23	2:C:171:LEU:H	1.85	0.41
2:C:549:ASP:OD1	3:D:750:PRO:HG2	2.20	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.81	0.41
3:D:746:LEU:H	3:D:746:LEU:HD12	1.86	0.41
3:D:905:ARG:NH1	3:D:910:ASN:OD1	2.54	0.41
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	2.02	0.41
1:G:69:SER:O	1:G:78:ILE:HG12	2.21	0.41
1:G:75:GLN:O	2:I:729:ALA:HB2	2.20	0.41
1:G:102:LEU:HD22	1:G:103:ASN:H	1.86	0.41
1:H:219:ARG:O	1:H:223:ILE:HG13	2.21	0.41
2:I:98:VAL:HG21	2:I:124:MET:HE3	2.03	0.41
3:J:24:LEU:HD13	3:J:24:LEU:HA	1.97	0.41
3:J:591:ILE:HG13	3:J:604:MET:HE2	2.02	0.41
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	2.02	0.41
2:C:62:TYR:CZ	2:C:476:LYS:HB3	2.56	0.41
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.90	0.41
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.35	0.41
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	2.03	0.41
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.21	0.41
2:C:1250:SER:OG	5:F:524:GLU:OE1	2.29	0.41
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.03	0.41
4:E:4:VAL:HG22	4:E:5:THR:HG23	2.03	0.41
5:F:94:THR:HG23	5:F:96:ASP:OD1	2.20	0.41
1:G:164:ASP:C	1:G:166:ARG:H	2.28	0.41
1:H:84:ASN:O	1:H:128:HIS:HE1	2.04	0.41
1:H:112:ALA:HB2	1:H:128:HIS:HB3	2.01	0.41
1:H:151:GLY:O	1:H:177:TYR:HD2	2.04	0.41
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.56	0.41
2:I:548:ARG:O	2:I:570:GLY:HA3	2.21	0.41
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.85	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.03	0.41
3:J:198:CYS:HA	3:J:221:ILE:HD13	2.03	0.41
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.21	0.41
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.74	0.41
5:L:249:ILE:O	5:L:252:LEU:HB3	2.21	0.41
5:L:454:VAL:HA	5:L:457:ILE:HD12	2.03	0.41
1:A:60:GLU:CD	1:A:143:ARG:HH21	2.29	0.41
2:C:515:MET:HE3	2:C:517:GLN:HB2	2.03	0.41
3:D:481:ARG:O	3:D:488:ASN:ND2	2.54	0.41
3:D:902:ASP:OD1	3:D:903:LEU:N	2.54	0.41
3:D:1181:ASP:HA	3:J:202:ARG:HD3	2.02	0.41
3:D:1266:ILE:HD12	3:D:1273:ASP:O	2.20	0.41
5:F:226:ALA:HA	5:F:229:VAL:HG22	2.03	0.41
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.84	0.41
2:I:169:LYS:O	2:I:170:VAL:HG22	2.21	0.41
2:I:840:SER:O	2:I:1047:LEU:N	2.54	0.41
3:J:141:PHE:HA	3:J:180:MET:HE2	2.03	0.41
3:J:481:ARG:O	3:J:488:ASN:ND2	2.54	0.41
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.54	0.41
1:B:73:GLY:CA	1:B:134:THR:HG22	2.51	0.40
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.36	0.40
2:C:555:TYR:HD2	6:C:2001:4OE:FAA	1.94	0.40
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	2.02	0.40
2:C:1262:LYS:HD3	2:C:1262:LYS:HA	1.82	0.40
3:D:1198:VAL:HB	3:D:1210:ILE:HA	2.03	0.40
1:G:172:LEU:HD12	1:G:172:LEU:H	1.85	0.40
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.40
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.51	0.40
3:J:30:ILE:HG23	3:J:243:PRO:HG3	2.02	0.40
3:J:502:PRO:HB2	3:J:507:VAL:HG12	2.04	0.40
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.21	0.40
3:J:902:ASP:OD1	3:J:903:LEU:N	2.54	0.40
5:L:470:MET:HE3	5:L:478:PRO:HB3	2.03	0.40
5:L:484:ALA:HB1	5:L:491:GLU:HB2	2.02	0.40
2:C:171:LEU:HD23	2:C:171:LEU:HA	1.92	0.40
2:C:589:THR:HA	2:C:590:PRO:HD3	1.94	0.40
2:C:925:SER:O	2:C:1056:VAL:HG13	2.22	0.40
3:D:190:LYS:HB2	3:D:190:LYS:HE2	1.89	0.40
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.56	0.40
1:H:48:LEU:HA	1:H:180:VAL:HG21	2.03	0.40
1:H:57:THR:O	1:H:173:VAL:HB	2.21	0.40
3:J:770:LEU:H	3:J:770:LEU:HD22	1.86	0.40
3:J:1100:PHE:HB2	3:J:1200:GLU:CD	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.88	0.40
5:L:525:ASP:CG	5:L:528:LEU:HB2	2.47	0.40
5:L:565:ILE:HG22	5:L:566:ASP:CG	2.46	0.40
5:L:583:THR:HG22	5:L:584:ARG:H	1.85	0.40
1:A:57:THR:O	1:A:173:VAL:HG22	2.21	0.40
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.04	0.40
2:C:1288:GLN:HB2	3:D:1356:LEU:HD23	2.03	0.40
3:D:697:MET:O	3:D:701:LEU:HB2	2.21	0.40
1:G:49:SER:OG	1:G:50:SER:N	2.54	0.40
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.61	0.40
2:I:812:PHE:CZ	3:J:503:SER:HB2	2.56	0.40
2:I:1099:ASN:HD21	3:J:505:ASP:CG	2.29	0.40
3:J:901:ARG:HA	3:J:908:ILE:HA	2.03	0.40
5:L:215:GLU:HG2	5:L:218:ARG:HH21	1.85	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.49	0.40
1:A:313:SER:O	1:A:316:MET:HG3	2.21	0.40
2:C:243:PRO:HB2	2:C:278:GLU:HG3	2.03	0.40
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.36	0.40
2:C:1119:MET:HE3	2:C:1204:LEU:HD13	2.04	0.40
3:D:34:SER:OG	3:D:104:HIS:ND1	2.29	0.40
3:D:466:MET:HE2	3:D:466:MET:HB3	1.99	0.40
3:D:810:THR:HG23	3:D:811:GLU:H	1.86	0.40
3:D:1162:ILE:HA	3:D:1203:ARG:HA	2.04	0.40
5:F:96:ASP:HA	5:F:97:PRO:HD2	1.93	0.40
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.86	0.40
1:G:225:ALA:O	1:G:228:LEU:HB2	2.21	0.40
1:H:73:GLY:CA	1:H:134:THR:HG22	2.50	0.40
2:I:742:TYR:CD2	2:I:743:PRO:HD2	2.57	0.40
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.56	0.40
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.02	0.40
2:I:1272:GLU:HG2	2:I:1276:TRP:CE2	2.56	0.40
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.56	0.40
3:J:161:THR:H	3:J:164:GLN:HB2	1.86	0.40
3:J:372:MET:HE2	3:J:372:MET:HB3	1.93	0.40
3:J:418:GLU:HG3	4:K:45:LYS:N	2.25	0.40
3:J:430:HIS:HA	3:J:921:GLN:HB3	2.02	0.40
3:J:749:LYS:HG3	3:J:751:ASP:HB3	2.04	0.40
5:L:582:VAL:CG2	5:L:586:ARG:HG2	2.51	0.40
1:A:207:THR:HG22	1:A:208:ASN:H	1.86	0.40
2:C:117:ILE:HG21	2:C:488:MET:HG2	2.04	0.40
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.21	0.40
2:C:1262:LYS:C	2:C:1264:GLN:H	2.28	0.40
3:D:363:LEU:HD12	3:D:450:HIS:CE1	2.56	0.40
3:D:706:VAL:HG12	3:D:715:LYS:HB3	2.04	0.40
5:F:119:ILE:O	5:F:123:ILE:HG13	2.21	0.40
1:G:57:THR:O	1:G:173:VAL:HG22	2.22	0.40
1:H:151:GLY:O	1:H:177:TYR:HB2	2.21	0.40
1:H:195:ARG:HB2	1:H:198:LEU:HD21	2.03	0.40
2:I:242:VAL:HA	2:I:243:PRO:HD3	1.94	0.40
2:I:453:ILE:HD12	2:I:587:LEU:HD21	2.04	0.40
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.04	0.40
3:J:119:SER:O	3:J:121:PRO:N	2.55	0.40
3:J:557:LYS:HB2	3:J:557:LYS:HE3	1.80	0.40
3:J:598:LYS:HA	3:J:601:ILE:HG22	2.03	0.40
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.54	0.40
5:L:343:LYS:O	5:L:347:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/335 (89%)	269 (90%)	20 (7%)	9 (3%)	3	26
1	B	212/335 (63%)	191 (90%)	18 (8%)	3 (1%)	9	39
1	G	222/335 (66%)	200 (90%)	16 (7%)	6 (3%)	4	28
1	H	212/335 (63%)	192 (91%)	17 (8%)	3 (1%)	9	39
2	C	1338/1342 (100%)	1236 (92%)	95 (7%)	7 (0%)	24	60
2	I	1338/1342 (100%)	1234 (92%)	98 (7%)	6 (0%)	30	65
3	D	1145/1407 (81%)	1050 (92%)	90 (8%)	5 (0%)	30	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	J	1311/1407 (93%)	1196 (91%)	112 (8%)	3 (0%)	43	75
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	481 (90%)	50 (9%)	1 (0%)	43	75
5	L	529/613 (86%)	481 (91%)	48 (9%)	0	100	100
All	All	7301/8246 (88%)	6682 (92%)	576 (8%)	43 (1%)	21	57

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
1	A	319	GLU
1	A	320	ASN
1	B	29	GLU
2	C	237	LEU
3	D	10	ALA
3	D	120	LEU
1	G	193	GLU
2	I	237	LEU
3	J	120	LEU
1	A	323	PRO
2	C	170	VAL
2	I	170	VAL
1	A	62	ASP
5	F	7	SER
1	G	62	ASP
1	H	29	GLU
1	H	30	PRO
1	A	196	THR
1	B	13	LEU
1	B	15	ASP
2	C	659	GLN
2	C	1136	GLN
3	D	710	ASP
1	G	196	THR
2	I	659	GLN
2	I	1136	GLN
3	J	710	ASP
1	A	167	PRO
1	A	178	SER

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Mol	Chain	Res	Type
2	C	697	LYS
3	D	747	MET
1	G	167	PRO
1	G	178	SER
1	H	193	GLU
2	I	697	LYS
2	C	1186	VAL
3	D	831	VAL
2	I	1186	VAL
3	J	831	VAL
1	A	14	VAL
1	G	14	VAL
2	C	1159	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	257/292 (88%)	240 (93%)	17 (7%)	15	40
1	B	184/292 (63%)	162 (88%)	22 (12%)	5	21
1	G	191/292 (65%)	178 (93%)	13 (7%)	14	39
1	H	183/292 (63%)	164 (90%)	19 (10%)	7	25
2	C	1155/1157 (100%)	1055 (91%)	100 (9%)	9	32
2	I	1154/1157 (100%)	1054 (91%)	100 (9%)	9	32
3	D	964/1168 (82%)	862 (89%)	102 (11%)	6	24
3	J	1106/1168 (95%)	997 (90%)	109 (10%)	7	27
4	E	72/75 (96%)	65 (90%)	7 (10%)	8	27
4	K	67/75 (89%)	59 (88%)	8 (12%)	5	21
5	F	426/540 (79%)	383 (90%)	43 (10%)	7	26
5	L	428/540 (79%)	386 (90%)	42 (10%)	7	27
All	All	6187/7048 (88%)	5605 (91%)	582 (9%)	8	29

All (582) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	26	VAL
1	A	35	PHE
1	A	54	CYS
1	A	64	VAL
1	A	65	LEU
1	A	74	VAL
1	A	129	VAL
1	A	133	LEU
1	A	173	VAL
1	A	207	THR
1	A	231	PHE
1	A	317	ARG
1	A	318	LEU
1	A	319	GLU
1	A	321	TRP
1	B	8	PHE
1	B	9	LEU
1	B	12	ARG
1	B	13	LEU
1	B	16	ILE
1	B	27	THR
1	B	31	LEU
1	B	43	LEU
1	B	54	CYS
1	B	58	GLU
1	B	60	GLU
1	B	64	VAL
1	B	65	LEU
1	B	75	GLN
1	B	92	VAL
1	B	101	THR
1	B	116	THR
1	B	133	LEU
1	B	144	ILE
1	B	160	HIS
1	B	183	ILE
1	B	186	ASN
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE

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Mol	Chain	Res	Type
2	C	85	CYS
2	C	91	THR
2	C	114	VAL
2	C	115	LYS
2	C	116	ASP
2	C	131	THR
2	C	182	SER
2	C	202	ARG
2	C	235	ASN
2	C	285	ILE
2	C	292	ILE
2	C	316	GLU
2	C	320	ASP
2	C	321	LEU
2	C	360	LEU
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	453	ILE
2	C	481	LEU
2	C	484	LEU
2	C	486	THR
2	C	493	ILE
2	C	512	SER
2	C	517	GLN
2	C	518	ASN
2	C	530	ILE
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	550	VAL
2	C	558	VAL
2	C	575	LEU
2	C	604	HIS
2	C	615	VAL
2	C	618	GLN
2	C	623	LEU
2	C	657	THR
2	C	660	VAL
2	C	672	GLU
2	C	692	THR
2	C	697	LYS

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Mol	Chain	Res	Type
2	C	699	LEU
2	C	705	GLU
2	C	706	ARG
2	C	714	VAL
2	C	724	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	782	VAL
2	C	788	SER
2	C	815	SER
2	C	817	LEU
2	C	819	SER
2	C	828	PHE
2	C	839	VAL
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	967	LEU
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	990	ASP
2	C	1002	LEU
2	C	1005	GLU
2	C	1006	GLU
2	C	1014	LEU
2	C	1040	ASP
2	C	1046	VAL
2	C	1082	ILE
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1141	LEU
2	C	1155	VAL
2	C	1161	LEU
2	C	1172	LEU
2	C	1174	GLU
2	C	1198	LEU

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Mol	Chain	Res	Type
2	C	1204	LEU
2	C	1210	ILE
2	C	1233	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1253	LEU
2	C	1254	VAL
2	C	1264	GLN
2	C	1265	PHE
2	C	1299	ASN
2	C	1326	LEU
2	C	1327	LEU
2	C	1342	GLU
3	D	11	GLN
3	D	13	LYS
3	D	18	ASP
3	D	20	ILE
3	D	46	TYR
3	D	71	LEU
3	D	79	LYS
3	D	83	VAL
3	D	92	VAL
3	D	95	THR
3	D	97	VAL
3	D	117	LEU
3	D	119	SER
3	D	120	LEU
3	D	169	LEU
3	D	175	GLU
3	D	194	LEU
3	D	217	LEU
3	D	244	VAL
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	256	ASP
3	D	311	ARG
3	D	324	LEU
3	D	356	THR
3	D	374	LEU
3	D	394	ILE
3	D	416	ILE

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Mol	Chain	Res	Type
3	D	474	LEU
3	D	501	VAL
3	D	506	VAL
3	D	507	VAL
3	D	513	MET
3	D	523	GLU
3	D	536	LEU
3	D	547	ARG
3	D	568	SER
3	D	593	ASN
3	D	594	GLN
3	D	615	LYS
3	D	641	ILE
3	D	660	GLU
3	D	677	GLU
3	D	678	ARG
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	740	LEU
3	D	746	LEU
3	D	749	LYS
3	D	754	ILE
3	D	757	THR
3	D	767	LEU
3	D	770	LEU
3	D	810	THR
3	D	826	ILE
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	860	ARG
3	D	867	GLN

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Mol	Chain	Res	Type
3	D	890	THR
3	D	897	HIS
3	D	908	ILE
3	D	913	GLU
3	D	918	ILE
3	D	928	THR
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1167	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1202	GLU
3	D	1209	VAL
3	D	1215	GLU
3	D	1221	LEU
3	D	1244	GLN
3	D	1251	LYS
3	D	1255	VAL
3	D	1272	SER
3	D	1274	PHE
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1307	LEU
3	D	1309	ILE
3	D	1327	GLU
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
4	E	13	ILE
4	E	28	ARG
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	27	VAL
5	F	44	ILE
5	F	45	ILE
5	F	50	ASP

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Mol	Chain	Res	Type
5	F	98	VAL
5	F	100	MET
5	F	118	ASP
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	244	THR
5	F	251	LYS
5	F	297	MET
5	F	305	LEU
5	F	306	PHE
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	429	THR
5	F	445	ASP
5	F	449	THR
5	F	454	VAL
5	F	479	THR
5	F	486	ARG
5	F	488	LEU
5	F	491	GLU
5	F	494	ILE
5	F	496	LYS
5	F	499	LYS
5	F	508	GLU
5	F	528	LEU
5	F	530	LEU
5	F	540	LEU
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	578	LYS
5	F	580	PHE
5	F	583	THR
5	F	586	ARG
5	F	600	HIS
5	F	606	VAL
5	F	612	ASP
1	G	9	LEU
1	G	13	LEU
1	G	26	VAL

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Mol	Chain	Res	Type
1	G	35	PHE
1	G	54	CYS
1	G	64	VAL
1	G	65	LEU
1	G	74	VAL
1	G	129	VAL
1	G	133	LEU
1	G	173	VAL
1	G	186	ASN
1	G	207	THR
1	H	13	LEU
1	H	16	ILE
1	H	27	THR
1	H	29	GLU
1	H	31	LEU
1	H	54	CYS
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	92	VAL
1	H	101	THR
1	H	105	SER
1	H	116	THR
1	H	133	LEU
1	H	139	SER
1	H	144	ILE
1	H	183	ILE
1	H	186	ASN
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	81	ASP
2	I	85	CYS
2	I	91	THR
2	I	114	VAL
2	I	115	LYS
2	I	116	ASP
2	I	131	THR
2	I	182	SER
2	I	202	ARG
2	I	235	ASN

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Mol	Chain	Res	Type
2	I	285	ILE
2	I	292	ILE
2	I	316	GLU
2	I	320	ASP
2	I	321	LEU
2	I	360	LEU
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	453	ILE
2	I	481	LEU
2	I	484	LEU
2	I	486	THR
2	I	493	ILE
2	I	512	SER
2	I	517	GLN
2	I	518	ASN
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	550	VAL
2	I	558	VAL
2	I	575	LEU
2	I	604	HIS
2	I	615	VAL
2	I	618	GLN
2	I	623	LEU
2	I	657	THR
2	I	660	VAL
2	I	672	GLU
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	705	GLU
2	I	706	ARG
2	I	714	VAL
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU

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Mol	Chain	Res	Type
2	I	782	VAL
2	I	788	SER
2	I	815	SER
2	I	817	LEU
2	I	819	SER
2	I	828	PHE
2	I	839	VAL
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	967	LEU
2	I	974	ARG
2	I	979	LEU
2	I	984	VAL
2	I	990	ASP
2	I	1002	LEU
2	I	1005	GLU
2	I	1006	GLU
2	I	1014	LEU
2	I	1040	ASP
2	I	1046	VAL
2	I	1082	ILE
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1141	LEU
2	I	1155	VAL
2	I	1161	LEU
2	I	1172	LEU
2	I	1174	GLU
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1253	LEU
2	I	1254	VAL
2	I	1264	GLN
2	I	1265	PHE

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Mol	Chain	Res	Type
2	I	1299	ASN
2	I	1326	LEU
2	I	1327	LEU
3	J	18	ASP
3	J	20	ILE
3	J	46	TYR
3	J	71	LEU
3	J	83	VAL
3	J	92	VAL
3	J	95	THR
3	J	97	VAL
3	J	117	LEU
3	J	119	SER
3	J	120	LEU
3	J	169	LEU
3	J	175	GLU
3	J	194	LEU
3	J	217	LEU
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	306	LEU
3	J	311	ARG
3	J	324	LEU
3	J	356	THR
3	J	374	LEU
3	J	394	ILE
3	J	416	ILE
3	J	474	LEU
3	J	501	VAL
3	J	506	VAL
3	J	507	VAL
3	J	510	LEU
3	J	513	MET
3	J	523	GLU
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	568	SER
3	J	593	ASN

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Mol	Chain	Res	Type
3	J	594	GLN
3	J	615	LYS
3	J	641	ILE
3	J	660	GLU
3	J	677	GLU
3	J	678	ARG
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	740	LEU
3	J	746	LEU
3	J	749	LYS
3	J	754	ILE
3	J	757	THR
3	J	767	LEU
3	J	810	THR
3	J	826	ILE
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	860	ARG
3	J	867	GLN
3	J	897	HIS
3	J	908	ILE
3	J	913	GLU
3	J	918	ILE
3	J	928	THR
3	J	931	THR
3	J	972	LYS
3	J	987	GLU
3	J	997	VAL
3	J	1017	VAL
3	J	1025	MET

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Mol	Chain	Res	Type
3	J	1042	ASP
3	J	1062	LEU
3	J	1063	ASP
3	J	1073	ASP
3	J	1113	VAL
3	J	1115	ILE
3	J	1155	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1202	GLU
3	J	1209	VAL
3	J	1215	GLU
3	J	1244	GLN
3	J	1251	LYS
3	J	1255	VAL
3	J	1272	SER
3	J	1274	PHE
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1307	LEU
3	J	1327	GLU
3	J	1332	LEU
3	J	1333	THR
3	J	1343	GLU
4	K	4	VAL
4	K	13	ILE
4	K	28	ARG
4	K	31	GLN
4	K	36	ASP
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	27	VAL
5	L	44	ILE
5	L	45	ILE
5	L	50	ASP
5	L	98	VAL
5	L	100	MET

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Mol	Chain	Res	Type
5	L	118	ASP
5	L	127	ILE
5	L	130	VAL
5	L	154	GLU
5	L	244	THR
5	L	251	LYS
5	L	297	MET
5	L	305	LEU
5	L	306	PHE
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	429	THR
5	L	445	ASP
5	L	449	THR
5	L	454	VAL
5	L	479	THR
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU
5	L	494	ILE
5	L	496	LYS
5	L	499	LYS
5	L	508	GLU
5	L	528	LEU
5	L	530	LEU
5	L	540	LEU
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	578	LYS
5	L	580	PHE
5	L	583	THR
5	L	586	ARG
5	L	600	HIS
5	L	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	128	HIS

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Mol	Chain	Res	Type
1	A	294	ASN
1	A	320	ASN
2	C	513	GLN
2	C	684	ASN
2	C	761	GLN
2	C	1017	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1257	GLN
2	C	1268	GLN
2	C	1288	GLN
2	C	1314	GLN
3	D	158	GLN
3	D	196	GLN
3	D	364	HIS
3	D	419	HIS
3	D	435	GLN
3	D	560	ASN
3	D	593	ASN
3	D	665	GLN
3	D	667	GLN
3	D	777	HIS
3	D	792	ASN
3	D	897	HIS
3	D	1295	ASN
3	D	1367	GLN
4	E	61	ASN
4	E	62	GLN
5	F	131	GLN
5	F	345	GLN
5	F	406	GLN
5	F	461	ASN
5	F	472	GLN
5	F	545	HIS
1	G	66	HIS
1	G	103	ASN
1	G	128	HIS
2	I	343	HIS
2	I	513	GLN
2	I	677	ASN
2	I	684	ASN

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Mol	Chain	Res	Type
2	I	761	GLN
2	I	1017	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1257	GLN
2	I	1288	GLN
2	I	1314	GLN
2	I	1324	ASN
3	J	158	GLN
3	J	196	GLN
3	J	364	HIS
3	J	419	HIS
3	J	435	GLN
3	J	560	ASN
3	J	593	ASN
3	J	665	GLN
3	J	667	GLN
3	J	777	HIS
3	J	792	ASN
3	J	897	HIS
3	J	954	ASN
3	J	1126	GLN
3	J	1367	GLN
4	K	60	ASN
4	K	61	ASN
5	L	128	ASN
5	L	406	GLN
5	L	461	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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	4OE	C	2001	-	25,25,25	4.48	6 (24%)	36,37,37	1.91	11 (30%)
6	4OE	I	2001	-	25,25,25	4.48	6 (24%)	36,37,37	1.92	11 (30%)

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	4OE	C	2001	-	-	6/14/14/14	0/3/3/3
6	4OE	I	2001	-	-	6/14/14/14	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	2001	4OE	CAT-CAV	-13.34	1.32	1.39
6	C	2001	4OE	CAT-CAV	-13.27	1.32	1.39
6	C	2001	4OE	CAS-CAT	-9.90	1.33	1.48
6	I	2001	4OE	CAS-CAT	-9.84	1.33	1.48
6	C	2001	4OE	CAR-CAV	-9.68	1.33	1.47
6	I	2001	4OE	CAR-CAV	-9.60	1.33	1.47
6	C	2001	4OE	NAO-NAN	-7.57	1.23	1.36
6	I	2001	4OE	NAO-NAN	-7.55	1.23	1.36
6	C	2001	4OE	CAL-CAT	-6.23	1.32	1.40
6	I	2001	4OE	CAL-CAT	-6.23	1.32	1.40
6	I	2001	4OE	CAW-CAU	-4.86	1.40	1.50
6	C	2001	4OE	CAW-CAU	-4.82	1.40	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	4OE	CAW-CAU-CAQ	-4.89	117.29	120.44
6	I	2001	4OE	CAW-CAU-CAQ	-4.88	117.30	120.44
6	I	2001	4OE	CAV-NAO-NAN	-4.13	108.58	112.55
6	C	2001	4OE	CAV-NAO-NAN	-4.08	108.63	112.55
6	I	2001	4OE	CAT-CAL-NAN	-3.61	106.38	111.34
6	C	2001	4OE	CAT-CAL-NAN	-3.58	106.42	111.34
6	I	2001	4OE	CAL-NAN-NAO	3.50	110.44	105.19
6	C	2001	4OE	CAL-NAN-NAO	3.48	110.41	105.19
6	I	2001	4OE	CAR-CAV-CAT	-2.90	127.65	131.29
6	C	2001	4OE	CAR-CAV-CAT	-2.89	127.67	131.29
6	I	2001	4OE	CAM-CAU-CAW	2.76	123.28	116.60
6	C	2001	4OE	CAM-CAU-CAW	2.73	123.20	116.60
6	C	2001	4OE	CAR-CAV-NAO	2.46	124.35	121.23
6	I	2001	4OE	CAR-CAV-NAO	2.41	124.29	121.23
6	C	2001	4OE	CAL-CAT-CAV	2.39	106.56	104.64
6	I	2001	4OE	CAL-CAT-CAV	2.38	106.55	104.64
6	I	2001	4OE	FAD-CAW-CAU	-2.25	108.65	112.65
6	C	2001	4OE	FAD-CAW-CAU	-2.24	108.67	112.65
6	C	2001	4OE	CAH-CAQ-CAU	-2.05	120.75	123.46
6	I	2001	4OE	CAG-CAP-CAF	-2.03	120.13	122.80
6	I	2001	4OE	CAH-CAQ-CAU	-2.03	120.78	123.46
6	C	2001	4OE	CAG-CAP-CAF	-2.01	120.16	122.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

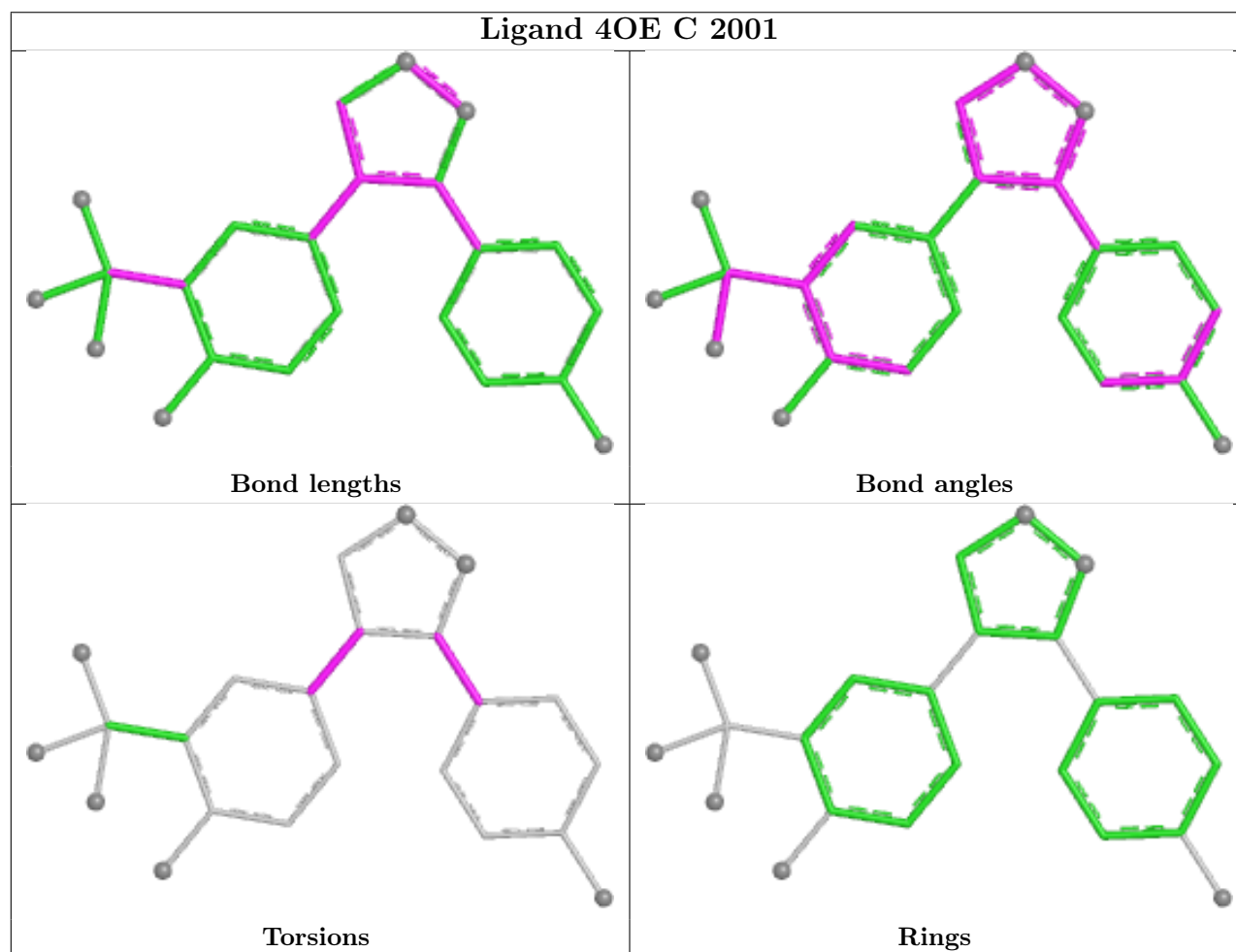
Mol	Chain	Res	Type	Atoms
6	C	2001	4OE	CAI-CAR-CAV-CAT
6	I	2001	4OE	CAI-CAR-CAV-CAT
6	C	2001	4OE	CAI-CAR-CAV-NAO
6	C	2001	4OE	CAJ-CAR-CAV-NAO
6	I	2001	4OE	CAI-CAR-CAV-NAO
6	I	2001	4OE	CAJ-CAR-CAV-NAO
6	C	2001	4OE	CAJ-CAR-CAV-CAT
6	I	2001	4OE	CAJ-CAR-CAV-CAT
6	C	2001	4OE	CAK-CAS-CAT-CAL
6	I	2001	4OE	CAK-CAS-CAT-CAL
6	C	2001	4OE	CAM-CAS-CAT-CAL
6	I	2001	4OE	CAM-CAS-CAT-CAL

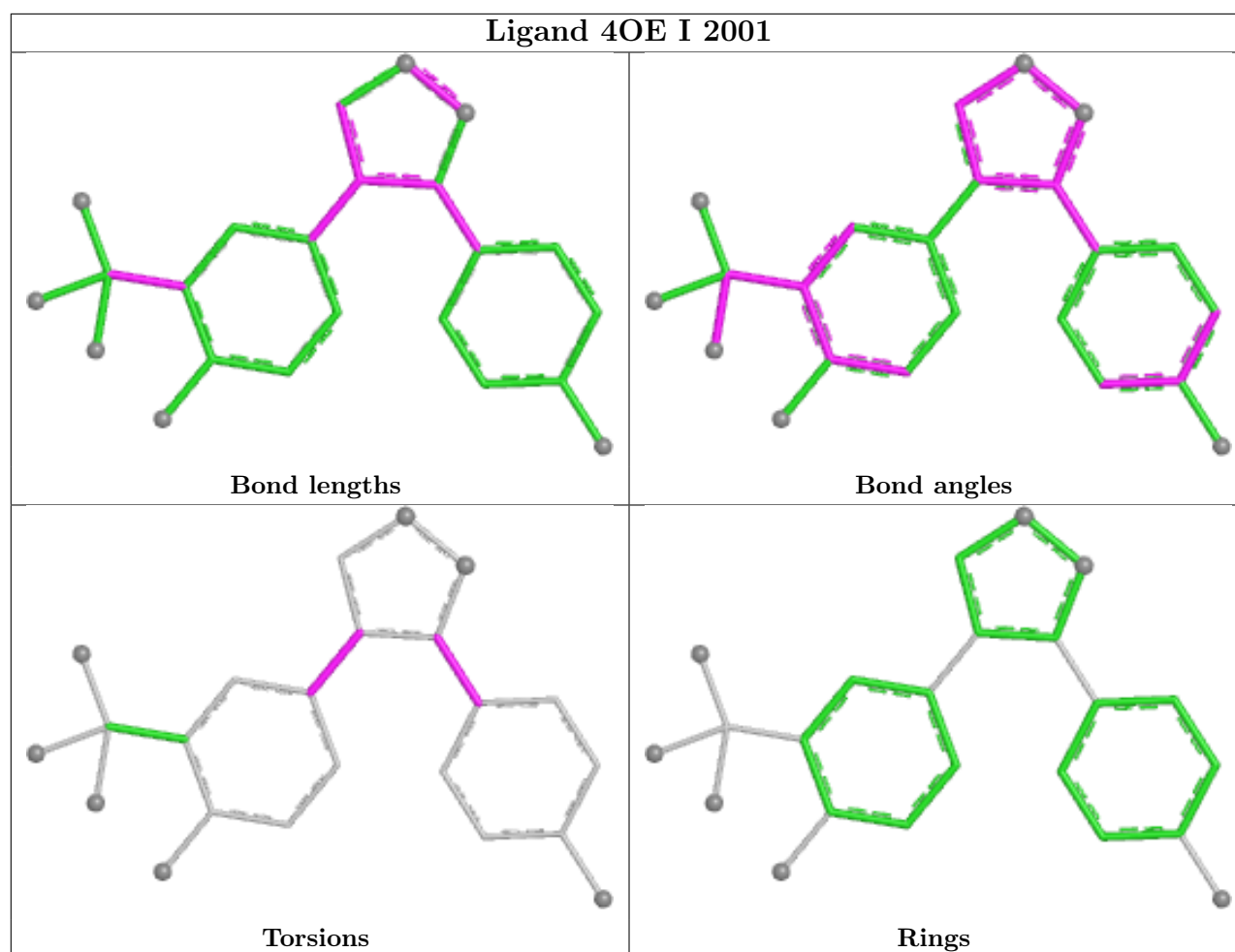
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2001	4OE	5	0
6	I	2001	4OE	4	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	302/335 (90%)	-0.47	4 (1%) 75 57	29, 105, 230, 394	0
1	B	216/335 (64%)	-0.32	1 (0%) 87 73	42, 129, 228, 299	0
1	G	224/335 (66%)	-0.47	4 (1%) 67 50	57, 116, 198, 279	0
1	H	216/335 (64%)	-0.28	1 (0%) 87 73	57, 136, 228, 269	0
2	C	1340/1342 (99%)	-0.32	18 (1%) 75 57	13, 89, 219, 379	0
2	I	1340/1342 (99%)	-0.37	14 (1%) 79 61	14, 112, 225, 339	0
3	D	1151/1407 (81%)	-0.38	10 (0%) 81 64	15, 70, 173, 283	0
3	J	1319/1407 (93%)	-0.38	7 (0%) 87 73	19, 94, 230, 319	0
4	E	89/91 (97%)	-0.54	0 100 100	27, 78, 123, 186	0
4	K	79/91 (86%)	-0.57	0 100 100	60, 124, 203, 243	0
5	F	542/613 (88%)	-0.31	5 (0%) 81 64	27, 158, 265, 368	0
5	L	539/613 (87%)	-0.40	3 (0%) 85 71	41, 153, 254, 312	0
All	All	7357/8246 (89%)	-0.37	67 (0%) 81 64	13, 105, 230, 394	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	56	VAL	5.0
2	I	882	ILE	4.4
1	G	231	PHE	4.2
2	C	206	ALA	3.8
5	F	259	PHE	3.7
2	C	433	ILE	3.4
3	J	904	ALA	3.4
2	C	205	PRO	3.3
2	I	471	VAL	3.2
2	I	931	VAL	3.2
5	L	134	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
5	F	256	PHE	3.1
1	G	39	LEU	3.0
3	D	117	LEU	2.9
2	I	347	ILE	2.9
2	C	47	TYR	2.9
2	I	1050	VAL	2.8
2	I	561	ILE	2.8
3	D	303	VAL	2.8
2	I	1052	VAL	2.7
2	C	52	ALA	2.7
2	C	453	ILE	2.6
3	J	1215	GLU	2.6
2	I	425	ILE	2.6
3	D	1184	ASP	2.6
2	C	364	VAL	2.6
1	A	205	MET	2.6
2	C	194	LEU	2.6
5	L	48	ILE	2.6
2	C	464	PHE	2.6
3	J	686	TRP	2.5
5	L	273	MET	2.5
3	D	306	LEU	2.5
2	I	224	PHE	2.5
5	F	463	LEU	2.5
2	C	21	VAL	2.5
3	D	244	VAL	2.5
3	J	269	TYR	2.5
3	J	324	LEU	2.4
2	C	179	TYR	2.4
2	C	347	ILE	2.4
2	I	875	ALA	2.4
1	G	90	VAL	2.4
1	H	217	ILE	2.4
2	C	292	ILE	2.4
1	A	231	PHE	2.3
1	A	216	ALA	2.3
2	C	679	ALA	2.3
3	J	217	LEU	2.3
2	I	928	VAL	2.3
2	I	1145	ILE	2.3
3	D	631	TYR	2.3
5	F	582	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	57	PHE	2.2
1	G	227	GLN	2.2
1	B	217	ILE	2.2
2	I	475	VAL	2.1
3	D	682	VAL	2.1
3	J	542	ALA	2.1
1	A	140	ILE	2.1
3	D	421	VAL	2.1
2	I	186	PHE	2.1
3	D	274	ASN	2.1
3	D	737	ILE	2.0
2	C	45	GLY	2.0
2	C	561	ILE	2.0
5	F	318	ALA	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](#)

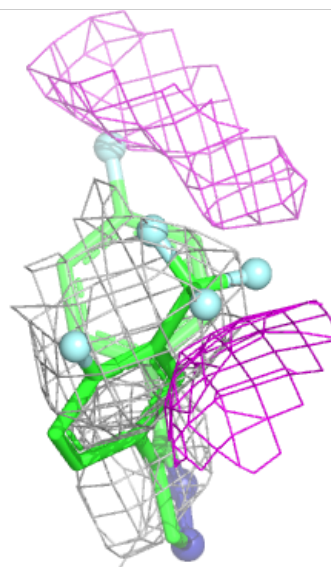
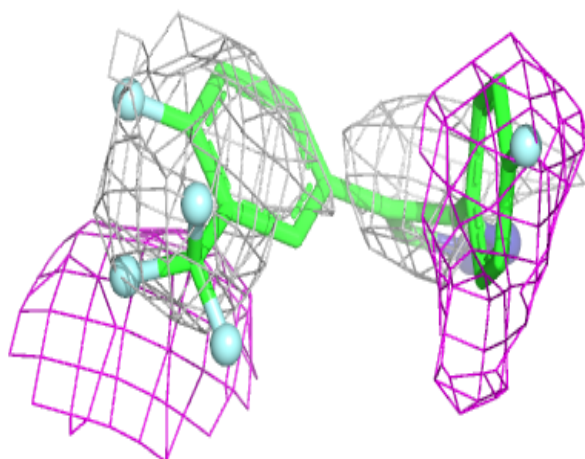
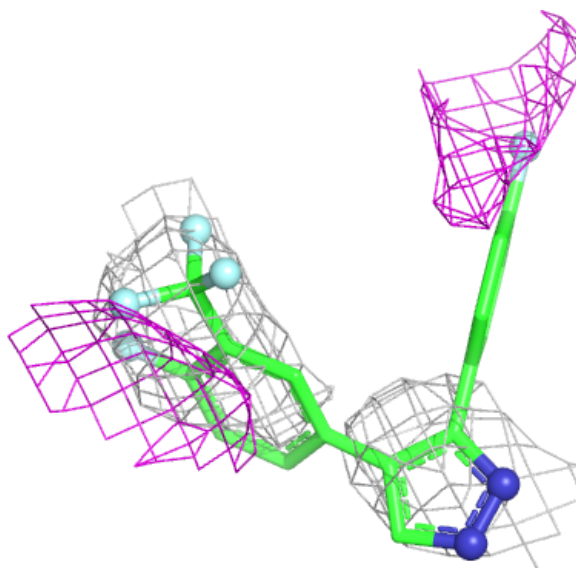
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

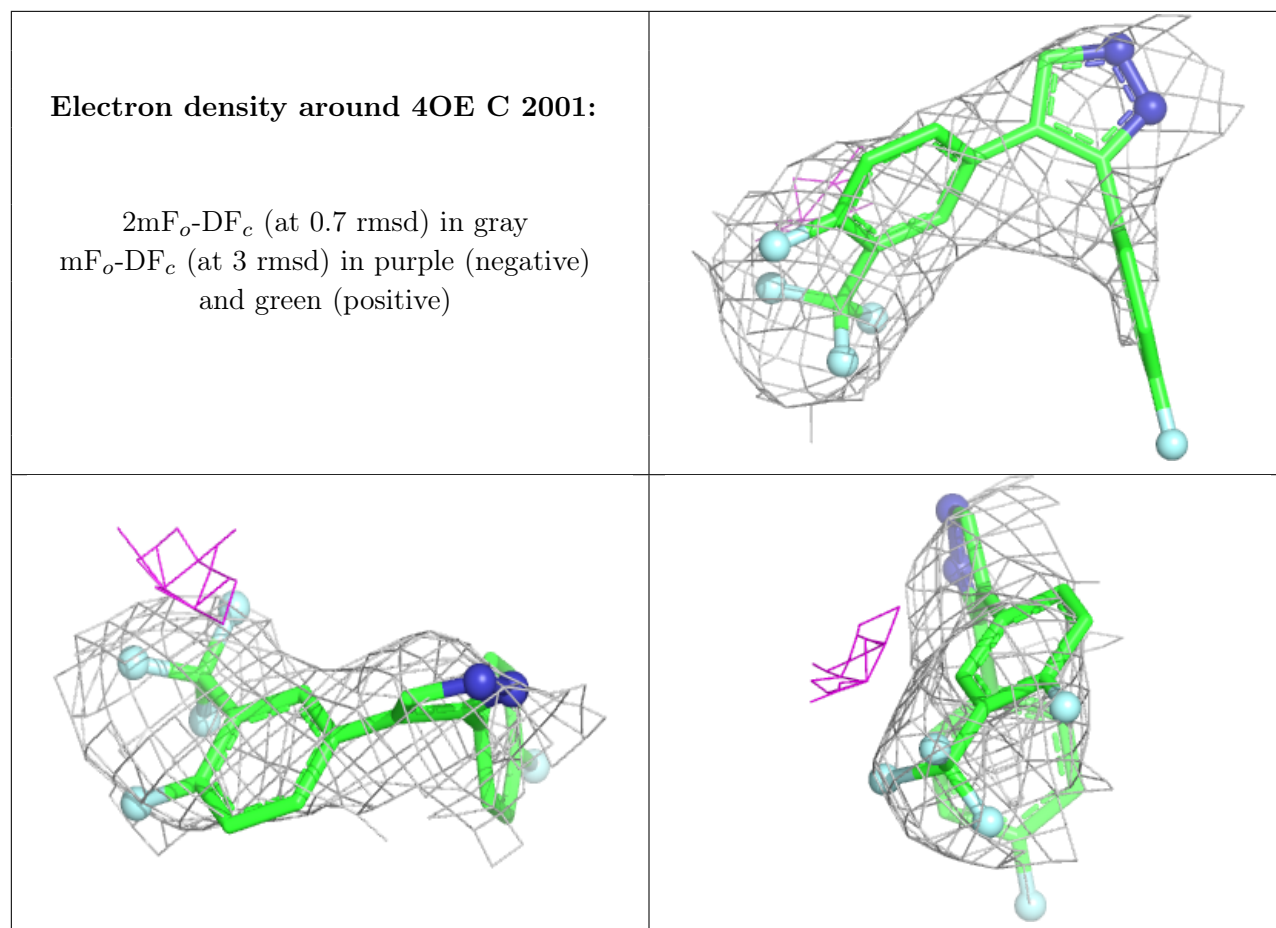
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	J	1501	1/1	0.50	0.18	69,69,69,69	0
6	4OE	I	2001	23/23	0.74	0.10	100,113,125,126	0
7	MG	D	1501	1/1	0.92	0.11	28,28,28,28	0
6	4OE	C	2001	23/23	0.92	0.06	48,74,93,102	0
8	ZN	D	1502	1/1	0.99	0.04	84,84,84,84	0
8	ZN	J	1502	1/1	0.99	0.06	94,94,94,94	0
8	ZN	D	1503	1/1	1.00	0.02	33,33,33,33	0
8	ZN	J	1503	1/1	1.00	0.04	54,54,54,54	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 4OE I 2001:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.