Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 11:18 PM EDT

PDB ID	:	4XSZ
Title	:	Crystal structure of CBR 9393 bound to Escherichia coli RNA polymerase holoenzyme
Authors	:	Bae, B.; Darst, S.A.
Deposited on	:	2015-01-22
Resolution	:	3.68 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:

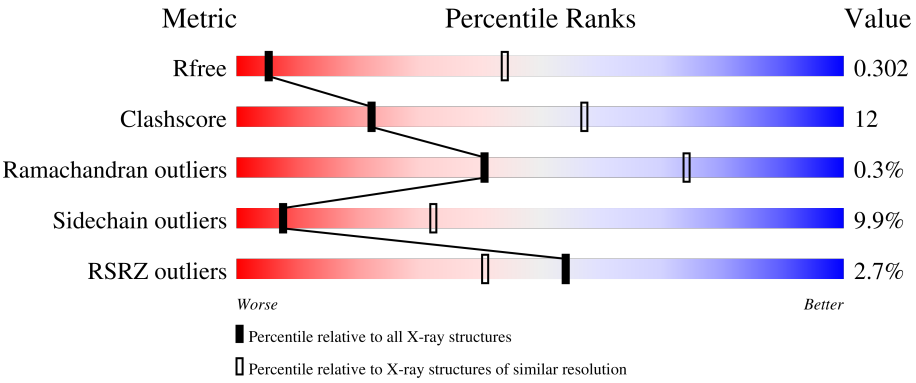
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.68 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}	130704	1013 (3.84-3.52)
Clashscore	141614	1070 (3.84-3.52)
Ramachandran outliers	138981	1036 (3.84-3.52)
Sidechain outliers	138945	1033 (3.84-3.52)
RSRZ outliers	127900	1471 (3.86-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	239	2% 64% 26% • 6%
1	B	239	4% 63% 26% • 8%
1	G	239	3% 67% 24% • 5%
1	H	239	7% 61% 27% • 9%
2	C	1342	% 66% 30% •

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Mol	Chain	Length	Quality of chain
2	I	1342	2% 67% 30%
3	D	1407	2% 55% 24% 17%
3	J	1407	2% 58% 26% 12%
4	E	91	74% 21%
4	K	91	65% 18% 13%
5	F	522	5% 62% 24% 10%
5	L	522	5% 63% 23% 10%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 55744 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

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

There are 20 discrepancies between the modelled and reference sequences:

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

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

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

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

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

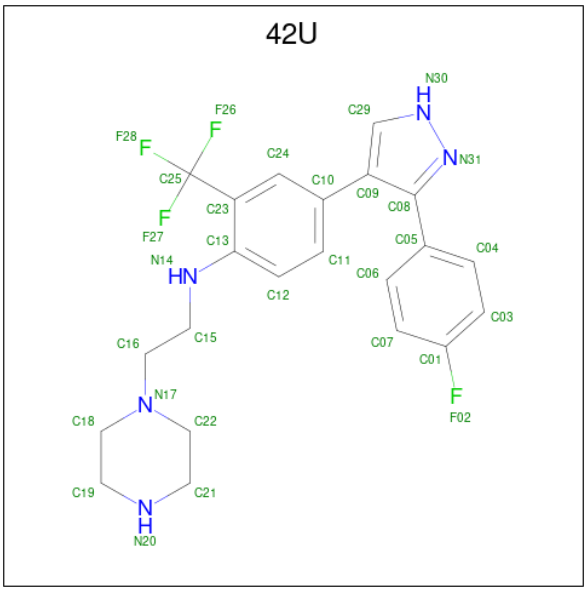
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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

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

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

- Molecule 6 is 4-[3-(4-fluorophenyl)-1H-pyrazol-4-yl]-N-[2-(piperazin-1-yl)ethyl]-2-(trifluoromethyl)aniline (three-letter code: 42U) (formula: $C_{22}H_{23}F_4N_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C F N 31 22 4 5	0	0
6	I	1	Total C F N 31 22 4 5	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

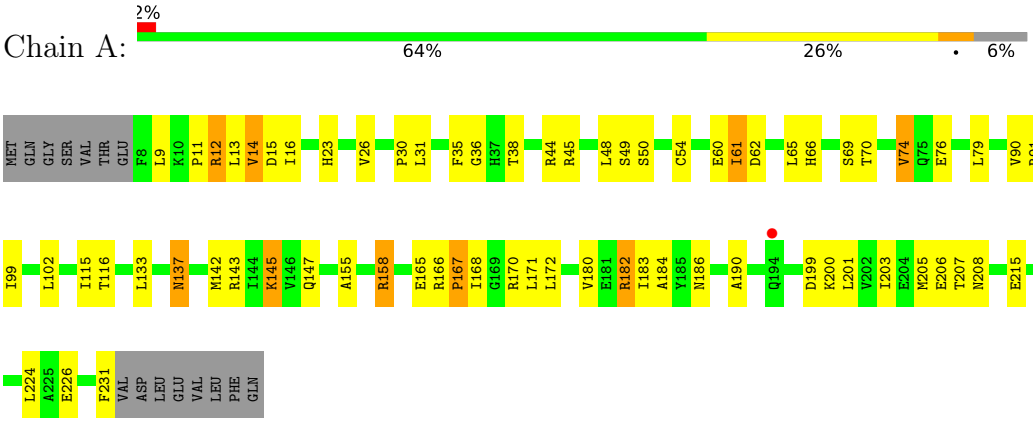
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	2	Total Zn 2 2	0	0
8	J	2	Total Zn 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

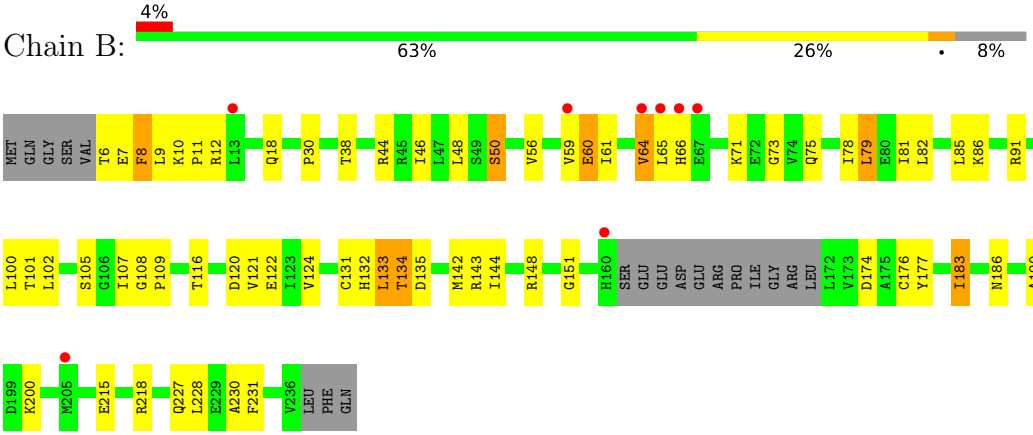
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



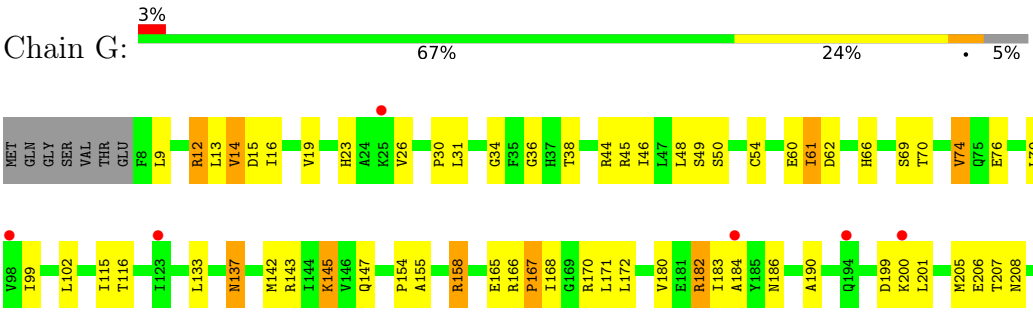
• Molecule 1: DNA-directed RNA polymerase subunit alpha

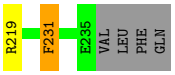
Chain B:



• Molecule 1: DNA-directed RNA polymerase subunit alpha

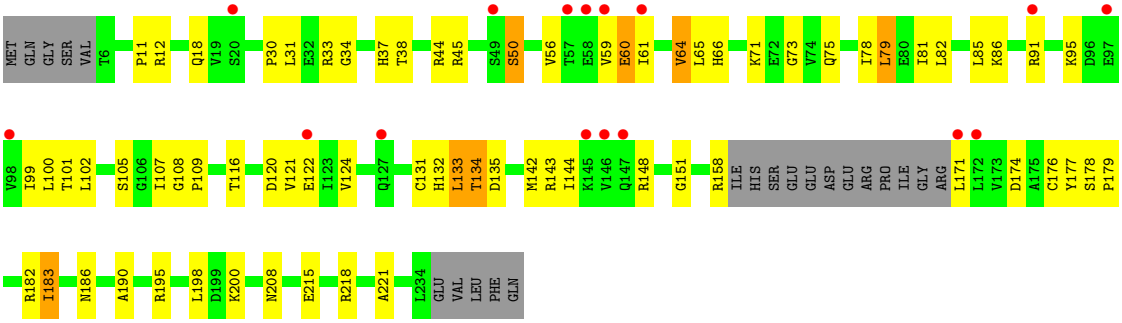
Chain G:





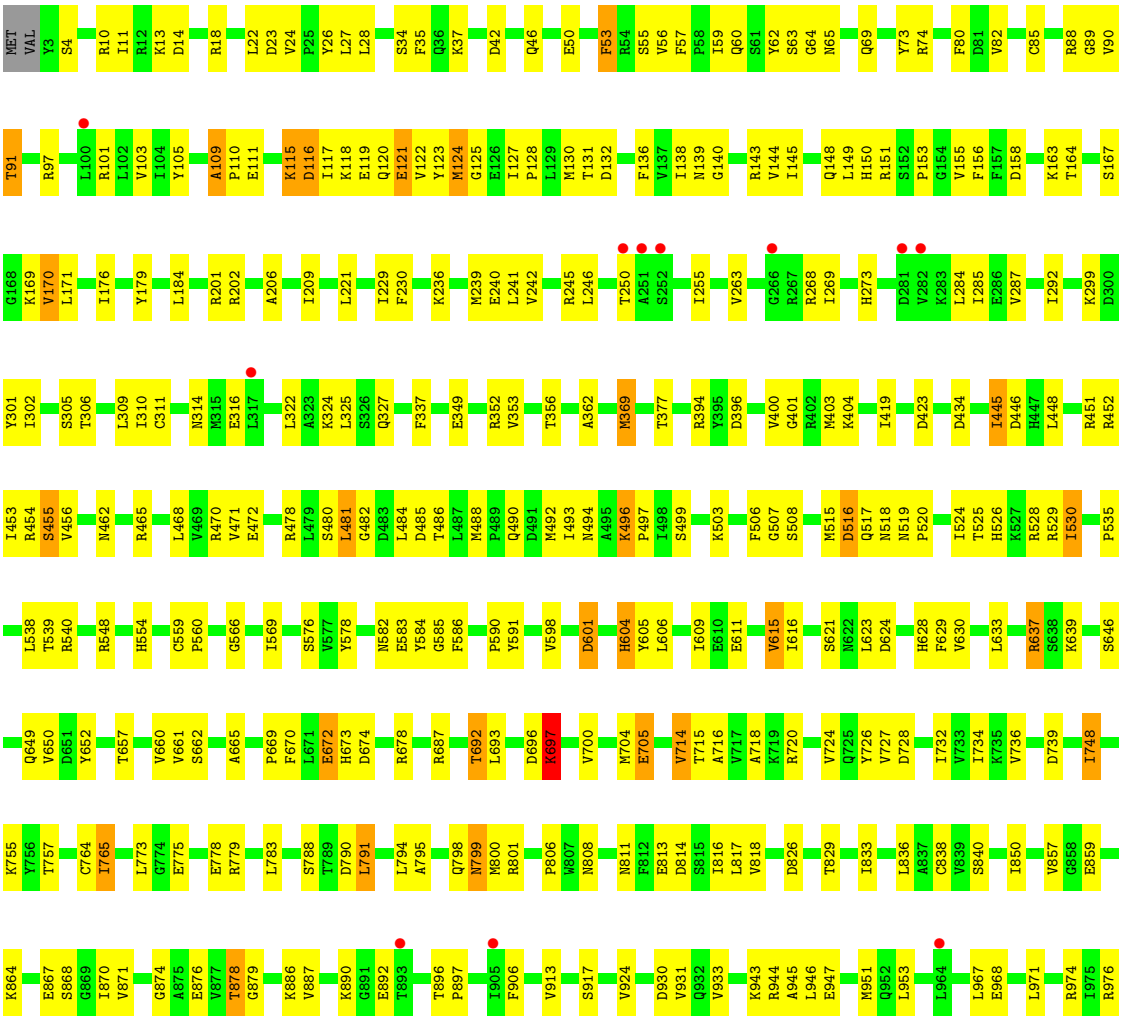
• Molecule 1: DNA-directed RNA polymerase subunit alpha

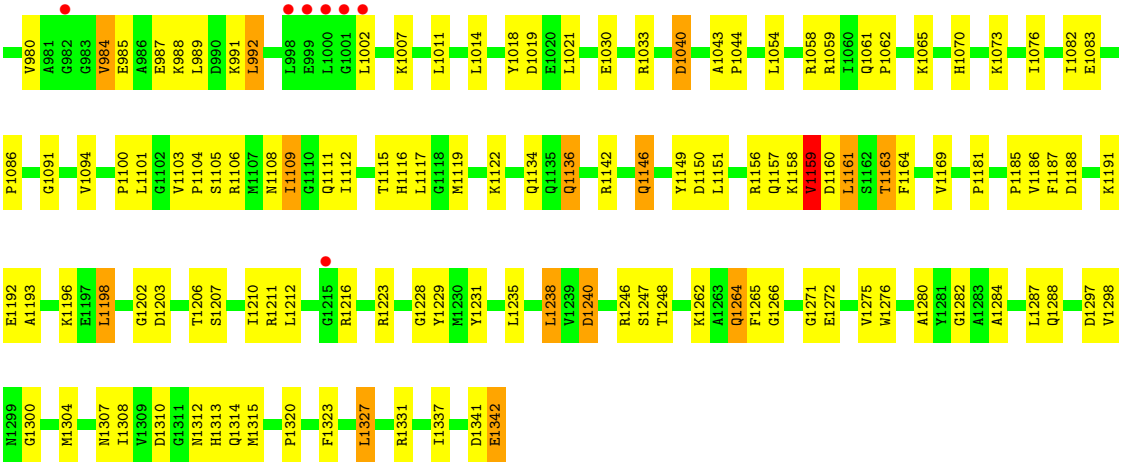
Chain H:



• Molecule 2: DNA-directed RNA polymerase subunit beta

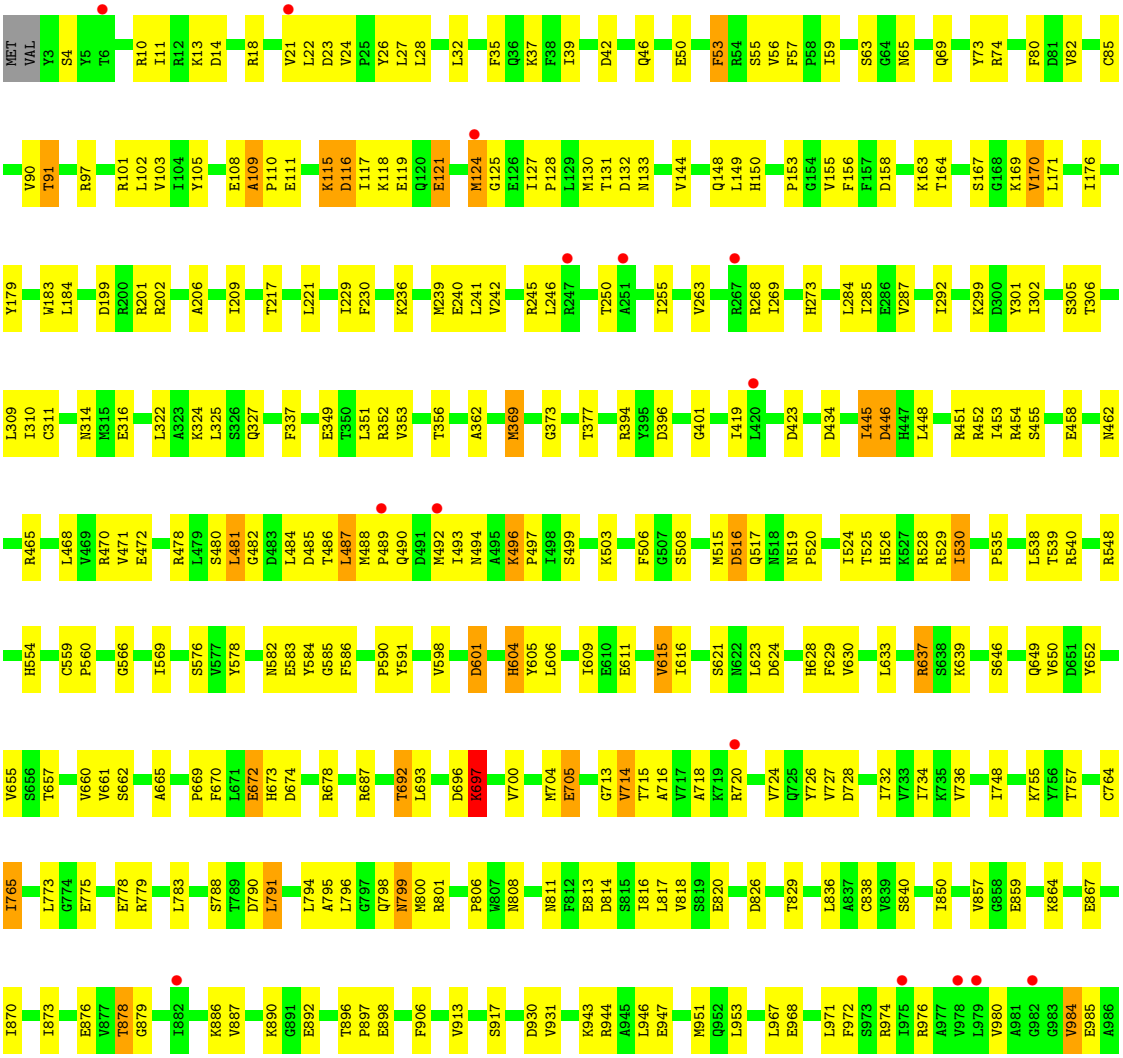
Chain C:



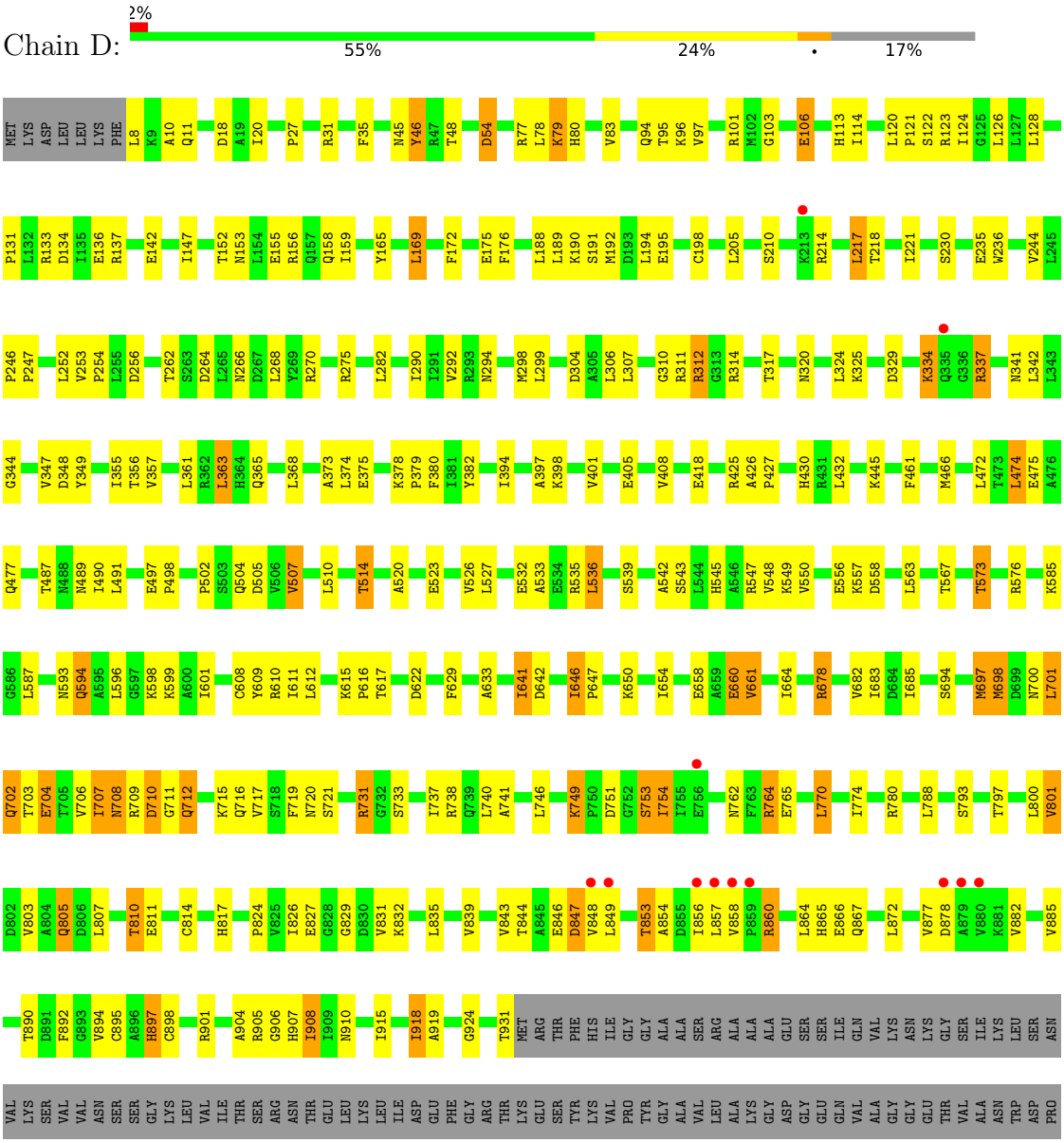


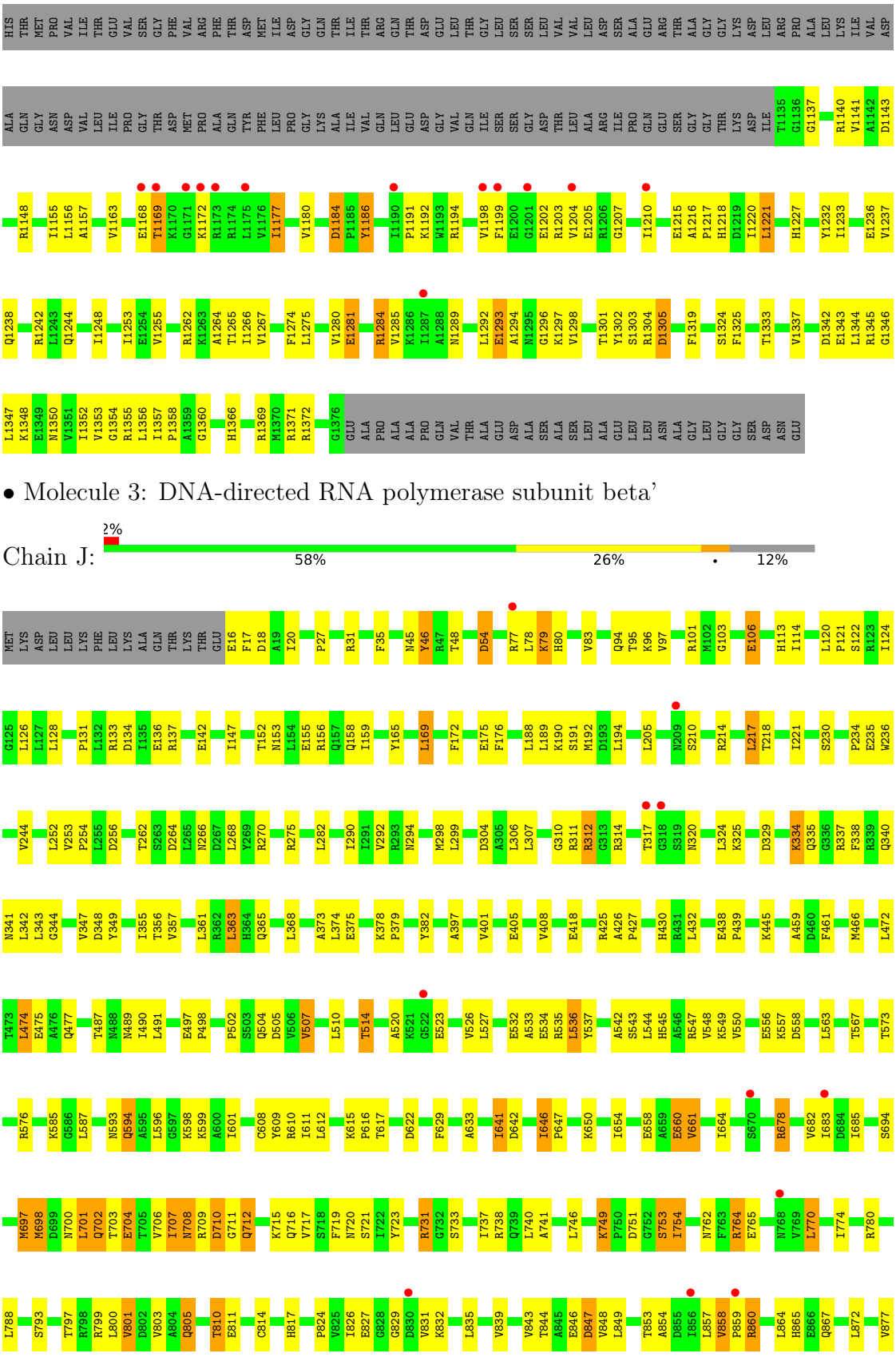
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain I:

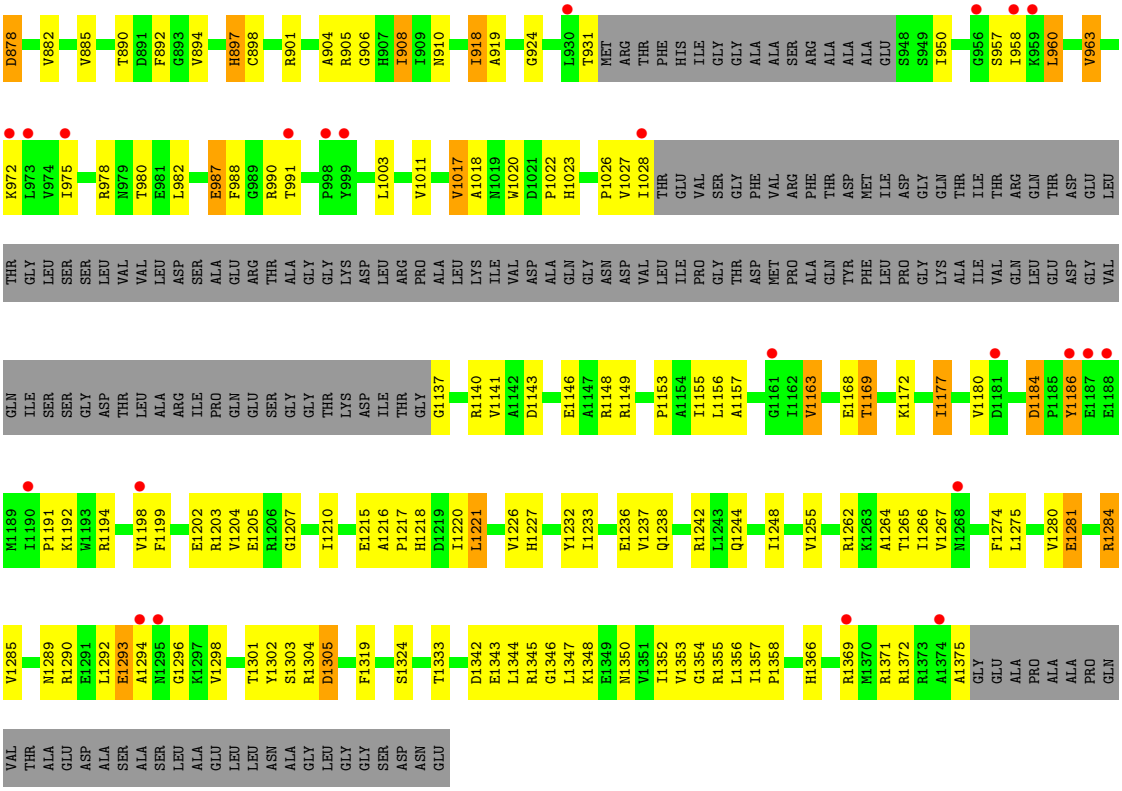


• Molecule 3: DNA-directed RNA polymerase subunit beta'



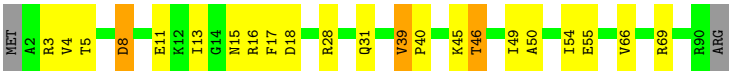


• Molecule 3: DNA-directed RNA polymerase subunit beta'



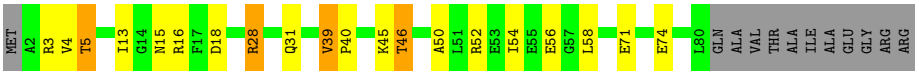
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



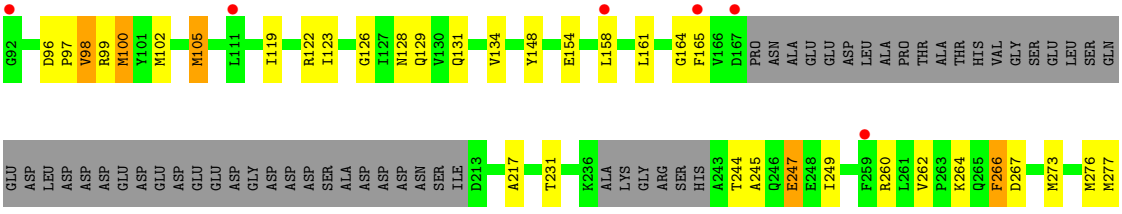
• Molecule 4: DNA-directed RNA polymerase subunit omega

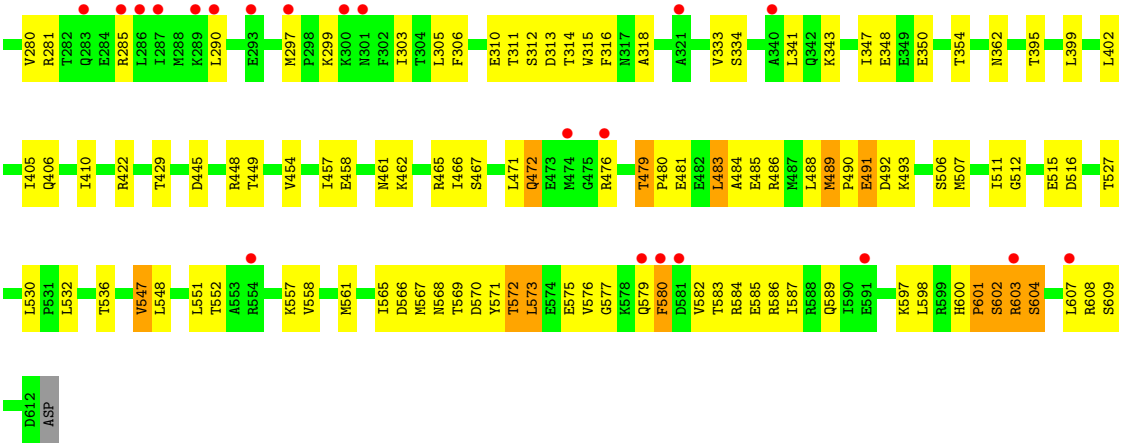
Chain K:



• Molecule 5: RNA polymerase sigma factor RpoD

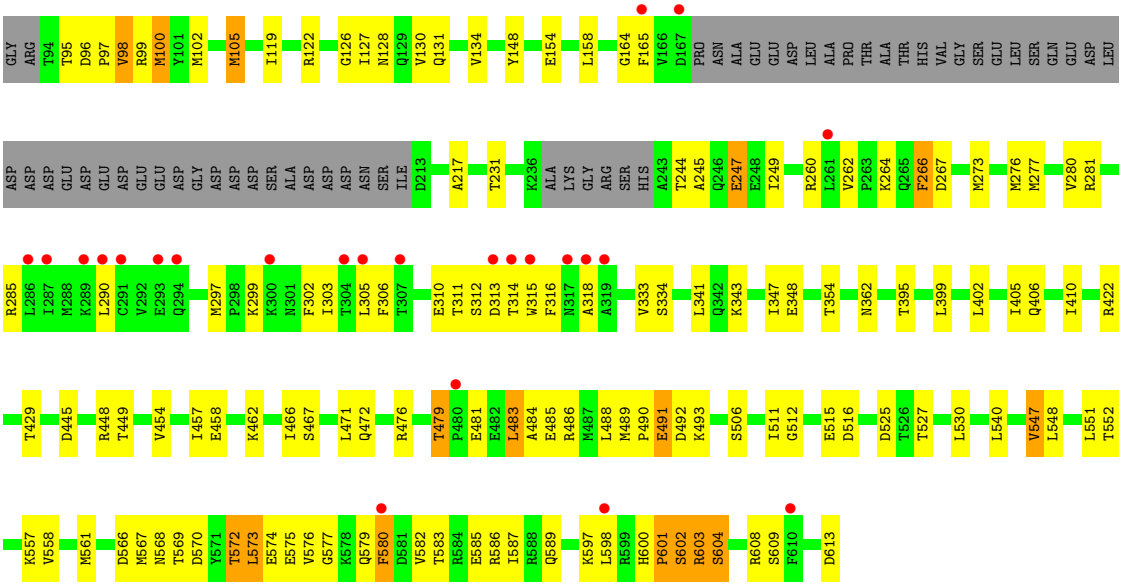
Chain F:





• Molecule 5: RNA polymerase sigma factor RpoD

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	184.44Å 206.33Å 309.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.93 – 3.68 39.93 – 3.68	Depositor EDS
% Data completeness (in resolution range)	88.5 (39.93-3.68) 88.5 (39.93-3.68)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 3.66Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.240 , 0.286 0.263 , 0.302	Depositor DCC
R_{free} test set	5687 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	139.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	55744	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 42U, MG, ZN

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	0.25	0/1751	0.54	0/2373
1	B	0.27	0/1707	0.53	0/2314
1	G	0.26	0/1771	0.56	0/2401
1	H	0.27	0/1686	0.51	0/2285
2	C	0.27	0/10739	0.52	0/14489
2	I	0.27	0/10735	0.51	0/14484
3	D	0.26	0/9246	0.51	0/12478
3	J	0.26	0/9785	0.51	0/13206
4	E	0.27	0/693	0.52	0/935
4	K	0.28	0/629	0.51	0/847
5	F	0.29	0/3873	0.51	1/5206 (0.0%)
5	L	0.29	0/3872	0.51	1/5205 (0.0%)
All	All	0.27	0/56487	0.52	2/76223 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
2	I	0	3
3	D	0	3
3	J	0	3
5	F	0	1
5	L	0	1
All	All	0	14

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	602	SER	N-CA-C	-6.49	93.48	111.00
5	L	602	SER	N-CA-C	-6.47	93.53	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	1161	LEU	Peptide
2	C	236	LYS	Peptide
3	D	1168	GLU	Peptide
3	D	1184	ASP	Peptide
3	D	1296	GLY	Peptide
5	F	601	PRO	Peptide
2	I	109	ALA	Peptide
2	I	1161	LEU	Peptide
2	I	236	LYS	Peptide
3	J	1168	GLU	Peptide
3	J	1184	ASP	Peptide
3	J	1296	GLY	Peptide
5	L	601	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1730	0	1756	49	0
1	B	1687	0	1700	47	0
1	G	1750	0	1764	45	0
1	H	1667	0	1689	55	0
2	C	10570	0	10582	277	0
2	I	10566	0	10576	256	0
3	D	9107	0	9309	251	0
3	J	9638	0	9853	261	0
4	E	691	0	695	19	0
4	K	627	0	634	10	0
5	F	3822	0	3885	91	0
5	L	3821	0	3884	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	31	0	23	0	0
6	I	31	0	23	0	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	55744	0	56373	1308	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (1308) 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	1.50	0.94
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.51	0.93
1:G:45:ARG:NH1	1:H:34:GLY:O	2.11	0.83
3:D:1372:ARG:HH21	3:J:854:ALA:HB3	1.42	0.83
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.62	0.81
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.63	0.81
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.63	0.80
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.62	0.79
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.65	0.78
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.65	0.78
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.65	0.78
3:D:418:GLU:HG3	4:E:45:LYS:H	1.48	0.78
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.67	0.77
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.65	0.77
3:J:128:LEU:HD23	3:J:192:MET:HE3	1.64	0.77
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.67	0.76
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.64	0.76
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.19	0.76
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.67	0.76
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.66	0.75
1:B:107:ILE:HG23	1:B:135:ASP:HA	1.69	0.75
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.67	0.75
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.67	0.74
3:J:418:GLU:HG3	4:K:45:LYS:H	1.52	0.74
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.68	0.74
1:H:107:ILE:HG23	1:H:135:ASP:HA	1.69	0.73
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.52	0.73
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.53	0.73
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.52	0.73
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.71	0.72
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.72	0.72
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.70	0.72
3:J:114:ILE:HD11	3:J:311:ARG:HB2	1.71	0.71
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.73	0.71
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.73	0.71
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.73	0.71
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.72	0.71
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.72	0.71
3:J:576:ARG:NH1	3:J:593:ASN:O	2.24	0.70
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.71	0.70
2:I:1142:ARG:HH11	2:I:1161:LEU:HD11	1.56	0.70
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.71	0.70
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	1.73	0.70
2:I:452:ARG:NH1	2:I:584:TYR:O	2.25	0.70
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.73	0.70
2:C:1142:ARG:HH11	2:C:1161:LEU:HD11	1.56	0.70
3:J:1266:ILE:HA	3:J:1302:TYR:HA	1.74	0.70
3:D:576:ARG:NH1	3:D:593:ASN:O	2.25	0.70
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.72	0.69
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.72	0.69
5:F:97:PRO:HA	5:F:100:MET:HG3	1.73	0.69
5:L:97:PRO:HA	5:L:100:MET:HG3	1.72	0.69
5:L:548:LEU:HD23	5:L:551:LEU:HD12	1.75	0.69
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.73	0.68
2:C:148:GLN:NE2	2:C:535:PRO:O	2.22	0.68
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.75	0.68
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.59	0.68
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.73	0.68
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.76	0.68
3:D:1266:ILE:HA	3:D:1302:TYR:HA	1.75	0.68
2:C:452:ARG:NH1	2:C:584:TYR:O	2.26	0.67
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	1.75	0.67
2:I:148:GLN:NE2	2:I:535:PRO:O	2.22	0.67
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.76	0.67
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.75	0.67
1:G:166:ARG:O	1:G:168:ILE:N	2.28	0.67
3:D:1297:LYS:HG2	3:J:1302:TYR:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:342:LEU:HD11	3:J:1324:SER:HB3	1.76	0.67
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.76	0.67
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.27	0.67
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.59	0.66
3:D:846:GLU:HA	3:D:860:ARG:HD3	1.75	0.66
1:A:166:ARG:O	1:A:168:ILE:N	2.28	0.66
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.77	0.66
3:J:846:GLU:HA	3:J:860:ARG:HD3	1.75	0.66
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.77	0.66
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.77	0.66
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.60	0.66
1:G:34:GLY:O	1:H:45:ARG:NH1	2.23	0.66
2:I:91:THR:HG21	2:I:503:LYS:HE2	1.78	0.66
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.78	0.66
2:I:829:THR:HA	2:I:1059:ARG:HA	1.79	0.65
3:D:556:GLU:HG2	3:D:558:ASP:HB2	1.78	0.65
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.78	0.65
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.61	0.65
3:J:378:LYS:NZ	3:J:382:TYR:OH	2.29	0.65
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.79	0.65
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.61	0.65
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.77	0.65
3:D:378:LYS:NZ	3:D:382:TYR:OH	2.29	0.65
2:C:91:THR:HG21	2:C:503:LYS:HE2	1.79	0.65
3:J:556:GLU:HG2	3:J:558:ASP:HB2	1.77	0.65
3:J:1203:ARG:HH12	3:J:1205:GLU:HG2	1.62	0.65
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.11	0.64
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.78	0.64
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.79	0.64
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.79	0.64
2:C:829:THR:HA	2:C:1059:ARG:HA	1.79	0.64
2:I:18:ARG:NH1	2:I:621:SER:O	2.31	0.64
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.62	0.64
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.31	0.64
5:L:277:MET:HG3	5:L:362:ASN:HD21	1.63	0.64
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.78	0.63
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.79	0.63
2:C:18:ARG:NH1	2:C:621:SER:O	2.31	0.63
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.80	0.63
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.31	0.63
3:D:1203:ARG:HH12	3:D:1205:GLU:HG2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.81	0.63
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.45	0.63
5:F:466:ILE:HB	5:F:483:LEU:HD23	1.81	0.63
2:I:452:ARG:NH2	2:I:458:GLU:OE2	2.27	0.63
5:F:277:MET:HG3	5:F:362:ASN:HD21	1.63	0.63
1:H:182:ARG:NH1	3:J:534:GLU:OE1	2.32	0.63
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.81	0.63
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.45	0.63
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.81	0.63
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.81	0.62
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.80	0.62
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.81	0.62
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.33	0.62
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.81	0.62
3:D:136:GLU:OE2	3:D:312:ARG:NH1	2.32	0.62
1:H:33:ARG:HD2	2:I:1081:PRO:HG3	1.82	0.62
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.81	0.62
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.81	0.62
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.65	0.62
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.81	0.62
3:J:136:GLU:OE2	3:J:312:ARG:NH1	2.32	0.62
5:L:128:ASN:HA	5:L:131:GLN:HE21	1.64	0.62
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.82	0.61
2:I:324:LYS:O	2:I:327:GLN:NE2	2.33	0.61
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.27	0.61
2:C:136:PHE:O	2:C:143:ARG:N	2.31	0.61
2:C:598:VAL:HG22	2:C:628:HIS:HE1	1.66	0.61
3:D:650:LYS:NZ	3:D:765:GLU:OE2	2.33	0.61
2:C:324:LYS:O	2:C:327:GLN:NE2	2.33	0.61
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.81	0.61
5:F:602:SER:OG	5:F:603:ARG:N	2.34	0.61
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.83	0.61
1:G:12:ARG:H	1:G:30:PRO:HD2	1.66	0.61
2:C:109:ALA:HB1	2:C:110:PRO:C	2.21	0.61
5:L:466:ILE:HB	5:L:483:LEU:HD23	1.81	0.60
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.82	0.60
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.82	0.60
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.82	0.60
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.83	0.60
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.82	0.60
3:J:963:VAL:HB	3:J:980:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.82	0.60
1:H:101:THR:H	1:H:116:THR:HG22	1.67	0.60
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.81	0.60
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.33	0.60
5:F:515:GLU:HG2	5:F:516:ASP:H	1.67	0.60
1:H:86:LYS:HD3	1:H:174:ASP:HB2	1.83	0.60
2:I:598:VAL:HG22	2:I:628:HIS:HE1	1.66	0.60
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.83	0.60
5:F:582:VAL:HG12	5:F:586:ARG:HG2	1.83	0.59
1:A:12:ARG:HG2	1:B:230:ALA:HB1	1.83	0.59
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.84	0.59
3:J:700:ASN:O	3:J:704:GLU:HB2	2.03	0.59
1:A:12:ARG:H	1:A:30:PRO:HD2	1.66	0.59
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.84	0.59
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.85	0.59
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.85	0.59
3:J:650:LYS:NZ	3:J:765:GLU:OE2	2.33	0.59
5:L:602:SER:OG	5:L:603:ARG:N	2.34	0.59
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.67	0.59
3:D:700:ASN:O	3:D:704:GLU:HB2	2.03	0.59
2:I:69:GLN:HE21	2:I:101:ARG:HD2	1.68	0.59
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.85	0.59
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.67	0.59
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.36	0.59
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.67	0.59
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.36	0.58
4:K:71:GLU:HA	4:K:74:GLU:HG3	1.85	0.58
3:D:152:THR:OG1	3:D:153:ASN:N	2.35	0.58
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.19	0.58
5:L:582:VAL:HG12	5:L:586:ARG:HG2	1.84	0.58
5:L:515:GLU:HG2	5:L:516:ASP:H	1.68	0.58
1:B:101:THR:H	1:B:116:THR:HG22	1.68	0.58
5:F:483:LEU:HD12	5:F:483:LEU:H	1.69	0.58
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.69	0.58
5:L:479:THR:HG23	5:L:481:GLU:H	1.68	0.58
1:A:23:HIS:HB2	1:A:205:MET:O	2.04	0.58
2:C:88:ARG:NE	2:C:1040:ASP:OD1	2.27	0.58
2:C:349:GLU:HA	2:C:352:ARG:HG3	1.86	0.58
1:G:23:HIS:HB2	1:G:205:MET:O	2.03	0.58
3:J:355:ILE:HD13	3:J:466:MET:HG3	1.84	0.58
2:C:400:VAL:HG21	2:C:452:ARG:CZ	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.69	0.58
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.86	0.58
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.86	0.58
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.86	0.57
2:I:349:GLU:HA	2:I:352:ARG:HG3	1.85	0.57
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.68	0.57
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.87	0.57
2:C:980:VAL:O	2:C:984:VAL:HB	2.05	0.57
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.85	0.57
2:C:868:SER:HB3	2:C:944:ARG:HB2	1.85	0.57
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.86	0.57
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.85	0.57
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.87	0.57
3:J:152:THR:OG1	3:J:153:ASN:N	2.36	0.57
3:J:682:VAL:O	3:J:685:ILE:HG12	2.05	0.57
3:J:1216:ALA:HB1	3:J:1218:HIS:HD2	1.70	0.57
1:H:151:GLY:O	1:H:177:TYR:HD2	1.88	0.57
2:I:813:GLU:HB2	3:J:461:PHE:HB2	1.87	0.57
3:J:210:SER:O	3:J:214:ARG:HG2	2.05	0.57
3:J:950:ILE:HG13	3:J:1020:TRP:HZ3	1.70	0.57
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.87	0.57
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.87	0.57
5:F:479:THR:HG23	5:F:481:GLU:H	1.69	0.57
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.87	0.57
5:L:483:LEU:HD12	5:L:483:LEU:H	1.70	0.57
3:D:741:ALA:O	3:D:762:ASN:ND2	2.38	0.56
1:H:99:ILE:HD11	1:H:143:ARG:HB3	1.87	0.56
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.87	0.56
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.87	0.56
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.88	0.56
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.86	0.56
1:B:151:GLY:O	1:B:177:TYR:HD2	1.88	0.56
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.87	0.56
3:D:682:VAL:O	3:D:685:ILE:HG12	2.05	0.56
3:D:1292:LEU:HD23	3:J:1226:VAL:HG11	1.87	0.56
3:D:1372:ARG:NH2	3:J:854:ALA:HB3	2.17	0.56
2:I:980:VAL:O	2:I:984:VAL:HB	2.04	0.56
2:I:598:VAL:HG22	2:I:628:HIS:CE1	2.41	0.56
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.88	0.56
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.87	0.56
1:A:61:ILE:HG22	1:A:62:ASP:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.88	0.56
2:C:598:VAL:HG22	2:C:628:HIS:CE1	2.40	0.56
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.71	0.56
3:D:210:SER:O	3:D:214:ARG:HG2	2.06	0.56
2:C:987:GLU:HG2	2:C:991:LYS:HE3	1.88	0.56
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.86	0.56
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.70	0.56
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.88	0.56
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.87	0.56
2:C:601:ASP:OD1	2:C:601:ASP:N	2.36	0.56
1:G:61:ILE:HG22	1:G:62:ASP:H	1.70	0.56
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.87	0.55
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.88	0.55
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.88	0.55
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.87	0.55
3:D:1293:GLU:OE1	3:D:1294:ALA:N	2.38	0.55
3:J:741:ALA:O	3:J:762:ASN:ND2	2.39	0.55
3:J:1293:GLU:OE1	3:J:1294:ALA:N	2.39	0.55
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.89	0.55
1:B:6:THR:O	1:B:6:THR:OG1	2.25	0.55
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.88	0.55
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.36	0.55
2:C:1223:ARG:NH1	3:D:721:SER:OG	2.36	0.55
1:H:60:GLU:OE2	1:H:143:ARG:NH1	2.40	0.55
3:J:335:GLN:HG2	3:J:343:LEU:HD11	1.87	0.55
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.88	0.55
2:I:560:PRO:O	3:J:780:ARG:NH2	2.39	0.55
1:A:224:LEU:HD22	1:B:228:LEU:HD11	1.87	0.55
2:I:601:ASP:OD1	2:I:601:ASP:N	2.37	0.55
5:F:561:MET:HA	5:F:567:MET:HE1	1.88	0.55
5:F:573:LEU:H	5:F:573:LEU:HD23	1.71	0.55
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.88	0.55
5:L:561:MET:HA	5:L:567:MET:HE1	1.87	0.55
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.89	0.55
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.88	0.55
2:C:560:PRO:O	3:D:780:ARG:NH2	2.40	0.55
2:I:1246:ARG:NH1	2:I:1266:GLY:HA2	2.21	0.55
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.88	0.55
1:B:60:GLU:OE2	1:B:143:ARG:NH1	2.40	0.55
2:I:987:GLU:HG2	2:I:991:LYS:HE3	1.88	0.55
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.89	0.54
2:C:115:LYS:HE3	2:C:116:ASP:H	1.72	0.54
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.89	0.54
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.89	0.54
2:C:1246:ARG:NH1	2:C:1266:GLY:HA2	2.21	0.54
2:I:115:LYS:HE3	2:I:116:ASP:H	1.72	0.54
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.88	0.54
3:J:698:MET:O	3:J:702:GLN:HB3	2.08	0.54
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.90	0.54
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.88	0.54
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.90	0.54
3:D:698:MET:O	3:D:702:GLN:HB3	2.08	0.54
3:D:1217:PRO:HG3	3:D:1232:TYR:HE2	1.73	0.54
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.32	0.54
5:L:573:LEU:HD23	5:L:573:LEU:H	1.73	0.54
3:J:514:THR:OG1	3:J:594:GLN:O	2.26	0.53
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.89	0.53
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.91	0.53
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.91	0.53
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.90	0.53
1:H:37:HIS:NE2	2:I:1216:ARG:HD2	2.24	0.53
2:I:27:LEU:HB2	2:I:524:ILE:HD11	1.90	0.53
5:L:488:LEU:H	5:L:488:LEU:HD12	1.74	0.53
2:I:616:ILE:HG13	2:I:652:TYR:HB2	1.90	0.53
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.88	0.53
3:J:54:ASP:OD1	3:J:54:ASP:N	2.42	0.53
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.73	0.53
2:C:1284:ALA:HB1	3:D:1356:LEU:HD22	1.91	0.53
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.90	0.53
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.90	0.53
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.90	0.53
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.91	0.53
3:J:1265:THR:O	3:J:1303:SER:N	2.38	0.53
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.90	0.53
1:A:14:VAL:HG22	1:A:15:ASP:H	1.73	0.53
2:I:1223:ARG:NH1	3:J:721:SER:OG	2.36	0.53
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.91	0.53
5:F:511:ILE:HG13	5:F:512:GLY:H	1.73	0.53
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.90	0.53
3:J:1217:PRO:HG3	3:J:1232:TYR:HE2	1.73	0.53
1:A:45:ARG:HG2	1:B:38:THR:HB	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:HD22	3:D:539:SER:HB3	1.91	0.53
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.91	0.53
3:D:514:THR:OG1	3:D:594:GLN:O	2.26	0.53
2:I:125:GLY:HA2	2:I:499:SER:HB2	1.90	0.53
3:D:356:THR:OG1	3:D:357:VAL:N	2.42	0.53
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.89	0.53
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.91	0.53
2:C:1304:MET:HE2	3:D:472:LEU:HB3	1.91	0.52
1:G:14:VAL:HG22	1:G:15:ASP:H	1.73	0.52
1:H:59:VAL:O	1:H:171:LEU:N	2.42	0.52
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.90	0.52
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.91	0.52
1:A:11:PRO:HD2	1:B:227:GLN:HA	1.90	0.52
1:A:218:ARG:NH1	1:B:231:PHE:O	2.43	0.52
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.90	0.52
2:C:124:MET:HB3	2:C:493:ILE:HD11	1.91	0.52
2:C:125:GLY:HA2	2:C:499:SER:HB2	1.91	0.52
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.74	0.52
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.90	0.52
2:C:27:LEU:HB2	2:C:524:ILE:HD11	1.90	0.52
3:D:707:ILE:HD11	3:D:716:GLN:HG2	1.90	0.52
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.91	0.52
2:C:155:VAL:HG23	2:C:176:ILE:HG12	1.91	0.52
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.90	0.52
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.41	0.52
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.92	0.52
5:F:488:LEU:HD12	5:F:488:LEU:H	1.73	0.52
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.91	0.52
3:J:1215:GLU:OE2	3:J:1215:GLU:N	2.43	0.52
4:K:31:GLN:HB2	4:K:46:THR:HG21	1.92	0.52
5:L:511:ILE:HG13	5:L:512:GLY:H	1.74	0.52
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.91	0.52
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.92	0.52
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.92	0.52
2:I:155:VAL:HG23	2:I:176:ILE:HG12	1.92	0.52
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.90	0.52
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.91	0.52
2:I:124:MET:HB3	2:I:493:ILE:HD11	1.91	0.52
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.91	0.52
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.09	0.52
2:C:151:ARG:CZ	2:C:445:ILE:HD11	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1288:GLN:HG2	2:C:1315:MET:HE1	1.91	0.52
3:D:54:ASP:N	3:D:54:ASP:OD1	2.42	0.52
2:I:170:VAL:HG23	2:I:171:LEU:N	2.25	0.52
2:C:122:VAL:HG23	5:F:472:GLN:HG3	1.92	0.52
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.75	0.52
1:G:44:ARG:HA	1:G:183:ILE:HG21	1.92	0.52
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.91	0.52
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.91	0.52
1:A:44:ARG:HA	1:A:183:ILE:HG21	1.91	0.52
1:B:134:THR:HG23	1:B:135:ASP:H	1.74	0.52
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.75	0.52
1:H:44:ARG:HG2	1:H:183:ILE:HD13	1.92	0.52
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.74	0.52
2:C:1142:ARG:NH1	2:C:1161:LEU:HD11	2.25	0.51
3:D:1215:GLU:N	3:D:1215:GLU:OE2	2.43	0.51
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.09	0.51
1:H:134:THR:HG23	1:H:135:ASP:H	1.75	0.51
2:I:301:TYR:HB2	2:I:311:CYS:SG	2.50	0.51
3:J:264:ASP:OD2	5:L:506:SER:OG	2.28	0.51
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.74	0.51
3:D:1216:ALA:HB1	3:D:1218:HIS:HD2	1.76	0.51
2:I:150:HIS:CD2	2:I:454:ARG:HE	2.29	0.51
3:J:527:LEU:HD22	3:J:533:ALA:HA	1.92	0.51
5:L:603:ARG:HH11	5:L:603:ARG:HA	1.75	0.51
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.42	0.51
2:C:548:ARG:HB3	2:C:569:ILE:O	2.10	0.51
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.92	0.51
2:C:808:ASN:H	3:D:633:ALA:HB2	1.75	0.51
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.93	0.51
5:F:603:ARG:HA	5:F:603:ARG:HH11	1.75	0.51
2:I:1284:ALA:HB1	3:J:1356:LEU:HD22	1.93	0.51
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.75	0.51
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.93	0.51
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.93	0.51
2:C:301:TYR:HB2	2:C:311:CYS:SG	2.50	0.51
3:D:847:ASP:OD1	3:D:847:ASP:N	2.40	0.51
2:I:548:ARG:HB3	2:I:569:ILE:O	2.11	0.51
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.92	0.51
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.74	0.51
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.93	0.51
5:F:280:VAL:HG22	5:F:347:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1160:ASP:HB2	2:C:1163:THR:OG1	2.11	0.51
1:G:16:ILE:HG23	1:G:26:VAL:HG12	1.93	0.51
2:I:1160:ASP:HB2	2:I:1163:THR:OG1	2.11	0.51
2:C:980:VAL:HA	2:C:984:VAL:HA	1.93	0.51
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.93	0.51
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.92	0.50
3:D:514:THR:HB	3:D:576:ARG:HG2	1.93	0.50
5:F:343:LYS:HD2	5:F:343:LYS:H	1.76	0.50
2:I:808:ASN:H	3:J:633:ALA:HB2	1.75	0.50
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.92	0.50
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.92	0.50
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.91	0.50
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.92	0.50
5:L:280:VAL:HG22	5:L:347:ILE:HD13	1.91	0.50
2:C:170:VAL:HG23	2:C:171:LEU:N	2.26	0.50
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.94	0.50
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.92	0.50
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.75	0.50
2:I:528:ARG:NH2	2:I:576:SER:O	2.44	0.50
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.92	0.50
2:I:980:VAL:HA	2:I:984:VAL:HA	1.93	0.50
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.93	0.50
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.47	0.50
1:H:81:ILE:O	1:H:85:LEU:HG	2.11	0.50
2:I:446:ASP:OD1	2:I:446:ASP:N	2.43	0.50
3:J:694:SER:OG	3:J:738:ARG:NE	2.45	0.50
3:D:264:ASP:OD2	5:F:506:SER:OG	2.29	0.50
1:G:137:ASN:OD1	1:G:137:ASN:N	2.45	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.93	0.50
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.92	0.50
1:B:44:ARG:HG2	1:B:183:ILE:HD13	1.93	0.50
2:C:1103:VAL:HG11	2:C:1112:ILE:HD11	1.92	0.50
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.92	0.50
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.11	0.50
3:J:958:ILE:HG23	3:J:982:LEU:HD11	1.93	0.50
5:L:343:LYS:H	5:L:343:LYS:HD2	1.77	0.50
1:A:137:ASN:OD1	1:A:137:ASN:N	2.44	0.50
2:C:757:THR:O	2:C:833:ILE:HD12	2.11	0.50
3:D:694:SER:OG	3:D:738:ARG:NE	2.45	0.50
3:D:1360:GLY:HA2	4:E:17:PHE:CE2	2.47	0.50
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:836:LEU:HD13	2:I:1054:LEU:HD13	1.93	0.50
1:A:172:LEU:HD12	1:A:172:LEU:H	1.75	0.50
1:B:73:GLY:O	1:B:134:THR:N	2.40	0.50
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.30	0.50
1:G:172:LEU:HD12	1:G:172:LEU:H	1.77	0.50
1:A:226:GLU:HG2	1:B:10:LYS:HE3	1.93	0.50
2:C:255:ILE:HB	2:C:263:VAL:HB	1.93	0.50
2:C:582:ASN:HB3	2:C:586:PHE:H	1.77	0.50
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.94	0.50
2:C:528:ARG:NH2	2:C:576:SER:O	2.45	0.49
2:C:1115:THR:HG22	2:C:1228:GLY:HA3	1.93	0.49
3:D:218:THR:HA	3:D:221:ILE:HG22	1.94	0.49
3:D:1221:LEU:HD11	3:D:1304:ARG:O	2.12	0.49
5:F:231:THR:HG23	5:F:249:ILE:HG12	1.94	0.49
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.93	0.49
1:B:81:ILE:O	1:B:85:LEU:HG	2.12	0.49
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.94	0.49
2:I:206:ALA:O	2:I:209:ILE:HG22	2.12	0.49
3:J:338:PHE:CB	3:J:343:LEU:HB2	2.42	0.49
5:L:551:LEU:HD11	5:L:598:LEU:HD11	1.94	0.49
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.46	0.49
3:D:856:ILE:HG13	3:J:1371:ARG:HD2	1.92	0.49
2:I:109:ALA:HB1	2:I:110:PRO:C	2.31	0.49
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.77	0.49
3:J:218:THR:HA	3:J:221:ILE:HG22	1.93	0.49
3:J:514:THR:HB	3:J:576:ARG:HG2	1.94	0.49
3:J:950:ILE:HG13	3:J:1020:TRP:CZ3	2.46	0.49
5:L:231:THR:HG23	5:L:249:ILE:HG12	1.94	0.49
1:B:134:THR:HG23	1:B:135:ASP:N	2.28	0.49
2:C:1149:TYR:HD1	2:C:1159:VAL:HG11	1.78	0.49
3:D:527:LEU:HD22	3:D:533:ALA:HA	1.93	0.49
3:D:770:LEU:H	3:D:770:LEU:HD22	1.78	0.49
4:E:50:ALA:O	4:E:54:ILE:HG12	2.11	0.49
2:I:674:ASP:OD2	2:I:1070:HIS:ND1	2.33	0.49
2:I:1146:GLN:NE2	2:I:1150:ASP:OD2	2.45	0.49
2:C:446:ASP:N	2:C:446:ASP:OD1	2.46	0.49
3:D:697:MET:O	3:D:701:LEU:HB2	2.12	0.49
3:D:1265:THR:O	3:D:1303:SER:N	2.39	0.49
5:F:547:VAL:HG21	5:F:607:LEU:HD13	1.94	0.49
5:F:548:LEU:HD11	5:F:565:ILE:HD13	1.94	0.49
2:I:255:ILE:HB	2:I:263:VAL:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.94	0.49
3:J:526:VAL:HG12	3:J:549:LYS:HB2	1.95	0.49
3:J:697:MET:O	3:J:701:LEU:HB2	2.12	0.49
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.12	0.49
2:C:34:SER:CB	2:C:455:SER:HB2	2.43	0.49
2:C:42:ASP:OD2	2:C:46:GLN:HB3	2.12	0.49
2:I:480:SER:HB3	2:I:481:LEU:HD22	1.94	0.49
5:F:490:PRO:HG2	5:F:493:LYS:HE3	1.95	0.49
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.77	0.49
3:J:847:ASP:OD1	3:J:847:ASP:N	2.39	0.49
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.95	0.49
3:D:654:ILE:O	3:D:658:GLU:HB2	2.13	0.49
1:H:108:GLY:O	1:H:133:LEU:HB2	2.13	0.49
2:I:582:ASN:HB3	2:I:586:PHE:H	1.77	0.49
2:I:1142:ARG:NH1	2:I:1161:LEU:HD11	2.26	0.49
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.95	0.49
2:C:206:ALA:O	2:C:209:ILE:HG22	2.13	0.49
2:C:886:LYS:H	2:C:917:SER:HB3	1.78	0.49
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.48	0.49
5:F:314:THR:O	5:F:318:ALA:HB3	2.13	0.49
2:I:1115:THR:HG22	2:I:1228:GLY:HA3	1.94	0.49
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.95	0.49
1:G:158:ARG:NH2	1:G:172:LEU:HD23	2.28	0.49
2:I:896:THR:HB	2:I:897:PRO:HD2	1.95	0.49
3:J:706:VAL:HG12	3:J:715:LYS:HB3	1.94	0.49
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.48	0.49
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.94	0.48
2:C:80:PHE:HB2	2:C:85:CYS:SG	2.53	0.48
2:C:403:MET:HG3	2:C:584:TYR:CZ	2.48	0.48
2:C:836:LEU:HD13	2:C:1054:LEU:HD13	1.94	0.48
3:D:77:ARG:HD2	3:D:78:LEU:H	1.78	0.48
1:H:73:GLY:O	1:H:134:THR:N	2.40	0.48
2:I:90:VAL:HG12	2:I:91:THR:H	1.78	0.48
3:J:598:LYS:O	3:J:601:ILE:HG22	2.13	0.48
5:L:490:PRO:HG2	5:L:493:LYS:HE3	1.95	0.48
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.93	0.48
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.48	0.48
1:H:82:LEU:HA	1:H:85:LEU:HD12	1.95	0.48
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.47	0.48
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.77	0.48
2:C:1271:GLY:HA2	3:D:344:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:202:ARG:HD3	2:I:369:MET:HG2	1.95	0.48
2:C:90:VAL:HG12	2:C:91:THR:H	1.78	0.48
2:C:480:SER:HB3	2:C:481:LEU:HD22	1.95	0.48
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.95	0.48
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.96	0.48
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.94	0.48
3:J:654:ILE:O	3:J:658:GLU:HB2	2.13	0.48
5:L:148:TYR:HE1	5:L:158:LEU:HD21	1.78	0.48
5:L:314:THR:O	5:L:318:ALA:HB3	2.13	0.48
1:B:101:THR:HG22	1:B:116:THR:HB	1.96	0.48
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.78	0.48
3:J:77:ARG:HD2	3:J:78:LEU:H	1.78	0.48
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.44	0.48
2:C:245:ARG:HG2	2:C:337:PHE:CZ	2.49	0.48
3:D:123:ARG:HD2	3:D:1337:VAL:HG11	1.94	0.48
1:G:182:ARG:H	1:G:206:GLU:HB3	1.79	0.48
2:I:1157:GLN:O	2:I:1158:LYS:HG2	2.13	0.48
3:J:709:ARG:C	3:J:711:GLY:H	2.16	0.48
5:L:244:THR:O	5:L:247:GLU:HG2	2.13	0.48
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.95	0.48
5:F:148:TYR:HE1	5:F:158:LEU:HD21	1.78	0.48
5:F:316:PHE:HZ	5:F:334:SER:HA	1.78	0.48
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.44	0.48
4:K:4:VAL:HG13	4:K:5:THR:HG23	1.96	0.48
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.95	0.48
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.96	0.48
2:C:1100:PRO:O	2:C:1104:PRO:HD3	2.14	0.48
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.95	0.48
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.47	0.48
3:D:526:VAL:HG12	3:D:549:LYS:HB2	1.95	0.48
2:I:499:SER:O	2:I:503:LYS:HB2	2.13	0.48
3:J:901:ARG:HA	3:J:908:ILE:HA	1.96	0.48
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.14	0.48
1:B:82:LEU:HA	1:B:85:LEU:HD12	1.96	0.48
1:B:108:GLY:O	1:B:133:LEU:HB2	2.14	0.48
2:C:1157:GLN:O	2:C:1158:LYS:HG2	2.13	0.48
3:D:347:VAL:HG12	3:D:348:ASP:O	2.14	0.48
3:D:598:LYS:O	3:D:601:ILE:HG22	2.13	0.48
1:H:134:THR:HG23	1:H:135:ASP:N	2.28	0.48
2:I:245:ARG:HG2	2:I:337:PHE:CZ	2.49	0.48
5:L:165:PHE:CZ	5:L:217:ALA:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.49	0.48
5:F:587:ILE:H	5:F:587:ILE:HD12	1.79	0.48
5:L:127:ILE:O	5:L:130:VAL:HG22	2.13	0.48
5:L:316:PHE:HZ	5:L:334:SER:HA	1.78	0.48
5:L:569:THR:OG1	5:L:570:ASP:N	2.47	0.48
5:L:587:ILE:HD12	5:L:587:ILE:H	1.79	0.48
1:B:95:LYS:HB2	1:B:120:ASP:OD2	2.15	0.47
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.45	0.47
2:C:202:ARG:HD3	2:C:369:MET:HG2	1.95	0.47
2:C:661:VAL:HB	2:C:665:ALA:HB3	1.96	0.47
2:C:871:VAL:C	2:C:944:ARG:HH12	2.17	0.47
2:I:886:LYS:H	2:I:917:SER:HB3	1.78	0.47
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.95	0.47
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	1.96	0.47
5:L:262:VAL:HG12	5:L:264:LYS:HG3	1.95	0.47
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.96	0.47
2:C:692:THR:OG1	2:C:693:LEU:N	2.47	0.47
2:I:696:ASP:O	2:I:697:LYS:HB3	2.14	0.47
2:I:1100:PRO:O	2:I:1104:PRO:HD3	2.14	0.47
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.96	0.47
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.48	0.47
3:J:770:LEU:HD22	3:J:770:LEU:H	1.79	0.47
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.96	0.47
5:L:164:GLY:O	5:L:260:ARG:HB2	2.14	0.47
5:L:281:ARG:HG2	5:L:285:ARG:HD2	1.95	0.47
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.96	0.47
2:C:1246:ARG:HH11	2:C:1266:GLY:HA2	1.78	0.47
5:F:244:THR:O	5:F:247:GLU:HG2	2.13	0.47
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.96	0.47
2:I:1149:TYR:CD1	2:I:1159:VAL:HG11	2.49	0.47
2:C:499:SER:O	2:C:503:LYS:HB2	2.14	0.47
3:D:709:ARG:C	3:D:711:GLY:H	2.16	0.47
5:F:165:PHE:CZ	5:F:217:ALA:HA	2.49	0.47
5:F:262:VAL:HG12	5:F:264:LYS:HG3	1.96	0.47
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.50	0.47
2:I:692:THR:OG1	2:I:693:LEU:N	2.47	0.47
2:I:878:THR:OG1	2:I:879:GLY:N	2.43	0.47
3:J:347:VAL:HG12	3:J:348:ASP:O	2.15	0.47
5:L:575:GLU:O	5:L:579:GLN:HG2	2.15	0.47
1:B:48:LEU:HD21	3:D:535:ARG:HG3	1.96	0.47
2:C:490:GLN:HG3	5:F:472:GLN:CD	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.49	0.47
2:I:726:TYR:CE2	2:I:728:ASP:HB2	2.50	0.47
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.15	0.47
1:A:182:ARG:H	1:A:206:GLU:HB3	1.80	0.47
3:D:394:ILE:HG23	5:F:536:THR:HG22	1.97	0.47
3:D:793:SER:O	3:D:797:THR:HG23	2.15	0.47
1:H:101:THR:HG22	1:H:116:THR:HB	1.96	0.47
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.95	0.47
3:J:797:THR:O	3:J:801:VAL:HG13	2.15	0.47
1:A:158:ARG:NH2	1:A:172:LEU:HD23	2.29	0.47
2:C:448:LEU:HA	2:C:451:ARG:HB2	1.97	0.47
2:C:696:ASP:O	2:C:697:LYS:HB3	2.13	0.47
2:C:816:ILE:HG22	2:C:818:VAL:HG23	1.97	0.47
2:I:35:PHE:CD2	2:I:130:MET:HB3	2.50	0.47
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.95	0.47
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.96	0.47
2:I:1149:TYR:HD1	2:I:1159:VAL:HG11	1.78	0.47
3:J:290:ILE:H	3:J:290:ILE:HD12	1.80	0.47
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.97	0.47
5:F:281:ARG:HG2	5:F:285:ARG:HD2	1.96	0.47
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.96	0.47
1:B:50:SER:HA	1:B:151:GLY:HA2	1.97	0.47
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.97	0.47
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.49	0.47
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.96	0.47
3:D:137:ARG:HG2	3:D:142:GLU:HB2	1.97	0.47
3:D:290:ILE:HD12	3:D:290:ILE:H	1.80	0.47
5:F:489:MET:H	5:F:489:MET:HG2	1.42	0.47
2:I:496:LYS:HB3	2:I:496:LYS:HE3	1.71	0.47
2:I:606:LEU:HD23	2:I:611:GLU:HA	1.97	0.47
3:J:131:PRO:HG2	3:J:134:ASP:HB2	1.97	0.47
3:J:810:THR:HG23	3:J:811:GLU:H	1.80	0.47
2:C:239:MET:O	2:C:284:LEU:HD12	2.15	0.47
2:C:878:THR:OG1	2:C:879:GLY:N	2.44	0.47
2:C:896:THR:HB	2:C:897:PRO:HD2	1.96	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.50	0.47
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.40	0.47
3:D:901:ARG:HA	3:D:908:ILE:HA	1.97	0.47
2:I:373:GLY:O	5:L:99:ARG:HD2	2.15	0.47
2:I:1253:LEU:HA	5:L:525:ASP:HB2	1.96	0.47
3:J:1346:GLY:O	3:J:1350:ASN:ND2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1116:HIS:CE1	3:D:641:ILE:H	2.30	0.46
2:C:1262:LYS:HB2	2:C:1264:GLN:HB3	1.96	0.46
2:C:1298:VAL:HG21	3:D:96:LYS:HE3	1.97	0.46
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.51	0.46
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.47	0.46
2:I:448:LEU:HA	2:I:451:ARG:HB2	1.97	0.46
2:I:1246:ARG:HH11	2:I:1266:GLY:HA2	1.79	0.46
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.50	0.46
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.96	0.46
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.15	0.46
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.80	0.46
2:I:1298:VAL:HG21	3:J:96:LYS:HE3	1.96	0.46
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.79	0.46
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.51	0.46
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.96	0.46
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.96	0.46
1:H:95:LYS:HB2	1:H:120:ASP:OD2	2.15	0.46
2:I:1271:GLY:HA2	3:J:344:GLY:HA2	1.96	0.46
3:J:475:GLU:OE1	4:K:28:ARG:NH1	2.44	0.46
3:J:843:VAL:HG11	3:J:897:HIS:O	2.16	0.46
5:L:348:GLU:HG2	5:L:354:THR:HA	1.98	0.46
1:B:71:LYS:HD2	1:B:71:LYS:HA	1.71	0.46
2:C:516:ASP:H	2:C:526:HIS:HD1	1.63	0.46
2:C:748:ILE:HD11	2:C:967:LEU:HA	1.96	0.46
2:C:1272:GLU:HB2	3:D:342:LEU:O	2.15	0.46
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.80	0.46
2:I:1061:GLN:NE2	2:I:1240:ASP:OD2	2.49	0.46
3:J:310:GLY:HA2	3:J:314:ARG:HG2	1.97	0.46
3:D:797:THR:O	3:D:801:VAL:HG13	2.15	0.46
5:F:164:GLY:O	5:F:260:ARG:HB2	2.14	0.46
5:F:348:GLU:HG2	5:F:354:THR:HA	1.98	0.46
2:I:516:ASP:H	2:I:526:HIS:HD1	1.64	0.46
3:J:122:SER:O	3:J:126:LEU:HG	2.16	0.46
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.98	0.46
2:C:1202:GLY:O	2:C:1203:ASP:HB2	2.16	0.46
3:D:839:VAL:HG13	3:D:882:VAL:HG21	1.98	0.46
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.96	0.46
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.15	0.46
3:D:1262:ARG:O	3:D:1280:VAL:HG23	2.15	0.46
5:F:551:LEU:HD11	5:F:598:LEU:HD11	1.97	0.46
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.98	0.46
2:I:1264:GLN:O	2:I:1264:GLN:HG2	2.16	0.46
3:J:502:PRO:HB2	3:J:507:VAL:HG12	1.97	0.46
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.96	0.46
2:C:494:ASN:HB3	2:C:497:PRO:HD2	1.98	0.46
2:C:520:PRO:HB3	2:C:714:VAL:HG21	1.97	0.46
5:F:245:ALA:O	5:F:249:ILE:HG13	2.15	0.46
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.97	0.46
2:I:1262:LYS:HB2	2:I:1264:GLN:HB3	1.96	0.46
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.97	0.46
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.49	0.46
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.98	0.46
3:D:133:ARG:HA	3:D:133:ARG:HD2	1.74	0.46
3:D:310:GLY:HA2	3:D:314:ARG:HG2	1.98	0.46
3:D:642:ASP:HA	3:D:764:ARG:HH21	1.81	0.46
1:H:33:ARG:NH2	2:I:820:GLU:OE2	2.47	0.46
3:J:31:ARG:NH2	3:J:106:GLU:OE2	2.41	0.46
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.97	0.46
3:J:557:LYS:HA	3:J:563:LEU:HA	1.98	0.46
5:L:245:ALA:O	5:L:249:ILE:HG13	2.16	0.46
3:D:557:LYS:HA	3:D:563:LEU:HA	1.97	0.46
3:D:708:ASN:HB3	3:D:712:GLN:O	2.16	0.46
3:D:810:THR:HG23	3:D:811:GLU:H	1.80	0.46
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.97	0.46
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.81	0.46
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.31	0.46
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.46
2:C:871:VAL:O	2:C:944:ARG:NH1	2.43	0.46
2:C:1061:GLN:NE2	2:C:1240:ASP:OD2	2.49	0.46
3:D:905:ARG:NH1	3:D:910:ASN:HD21	2.14	0.46
5:F:569:THR:OG1	5:F:570:ASP:N	2.48	0.46
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.98	0.46
3:J:708:ASN:HB3	3:J:712:GLN:O	2.16	0.46
3:J:1184:ASP:O	3:J:1186:TYR:N	2.49	0.46
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.49	0.46
1:A:66:HIS:CD2	2:C:874:GLY:HA2	2.50	0.45
1:B:61:ILE:HB	1:B:64:VAL:O	2.15	0.45
2:C:606:LEU:HD23	2:C:611:GLU:HA	1.97	0.45
2:C:1327:LEU:HD23	2:C:1337:ILE:HG23	1.98	0.45
3:D:1184:ASP:O	3:D:1186:TYR:N	2.49	0.45
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:724:VAL:HG23	2:I:775:GLU:O	2.16	0.45
2:I:1202:GLY:O	2:I:1203:ASP:HB2	2.16	0.45
5:L:481:GLU:O	5:L:484:ALA:HB3	2.16	0.45
2:C:176:ILE:HB	2:C:184:LEU:HB3	1.97	0.45
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.56	0.45
2:C:864:LYS:NZ	2:C:876:GLU:O	2.49	0.45
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.98	0.45
2:C:1276:TRP:CE2	3:D:801:VAL:HG21	2.51	0.45
3:D:430:HIS:CD2	3:D:432:LEU:HB2	2.51	0.45
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.31	0.45
2:I:1320:PRO:HG2	3:J:1354:GLY:HA3	1.98	0.45
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.50	0.45
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.45
3:J:661:VAL:HG12	3:J:685:ILE:HD11	1.98	0.45
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.98	0.45
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	1.98	0.45
2:C:1247:SER:HB3	3:D:375:GLU:O	2.16	0.45
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.97	0.45
3:D:1264:ALA:HA	3:D:1305:ASP:HB2	1.99	0.45
5:F:481:GLU:O	5:F:484:ALA:HB3	2.16	0.45
5:F:511:ILE:HD12	5:F:511:ILE:HA	1.84	0.45
2:I:1116:HIS:CE1	3:J:641:ILE:HB	2.52	0.45
3:J:430:HIS:CD2	3:J:432:LEU:HB2	2.51	0.45
3:J:749:LYS:HG3	3:J:753:SER:O	2.16	0.45
2:C:229:ILE:HB	2:C:240:GLU:HB2	1.98	0.45
2:C:992:LEU:H	2:C:992:LEU:HD23	1.81	0.45
2:C:1264:GLN:O	2:C:1264:GLN:HG2	2.16	0.45
3:D:282:LEU:HD21	5:F:410:ILE:HG12	1.98	0.45
2:I:705:GLU:HB2	2:I:794:LEU:HB3	1.99	0.45
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.56	0.45
3:J:266:ASN:O	3:J:270:ARG:HB2	2.16	0.45
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.16	0.45
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.47	0.45
1:H:61:ILE:HB	1:H:64:VAL:O	2.16	0.45
1:H:109:PRO:HB3	1:H:132:HIS:HD2	1.81	0.45
2:I:37:LYS:HA	2:I:37:LYS:HD3	1.68	0.45
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.81	0.45
3:J:137:ARG:HG2	3:J:142:GLU:HB2	1.97	0.45
1:B:102:LEU:HD12	1:B:142:MET:HG2	1.99	0.45
3:D:131:PRO:HG2	3:D:134:ASP:HB2	1.97	0.45
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:312:SER:OG	5:F:313:ASP:N	2.50	0.45
2:I:1276:TRP:CE2	3:J:801:VAL:HG21	2.52	0.45
2:I:1327:LEU:HD23	2:I:1337:ILE:HG23	1.98	0.45
1:A:207:THR:HG22	1:A:208:ASN:H	1.82	0.45
2:C:109:ALA:HB1	2:C:111:GLU:HA	1.99	0.45
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.76	0.45
2:C:404:LYS:HD3	2:C:586:PHE:CE1	2.52	0.45
3:D:266:ASN:O	3:D:270:ARG:HB2	2.16	0.45
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.97	0.45
1:H:50:SER:HA	1:H:151:GLY:HA2	1.98	0.45
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.74	0.45
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.52	0.45
5:L:572:THR:O	5:L:576:VAL:HG23	2.17	0.45
1:A:65:LEU:HB3	2:C:874:GLY:HA3	1.98	0.45
2:C:123:TYR:HB3	5:F:472:GLN:HB2	1.99	0.45
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.52	0.45
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.15	0.45
3:D:397:ALA:O	3:D:401:VAL:HG13	2.17	0.45
4:E:8:ASP:O	4:E:11:GLU:HB2	2.17	0.45
5:F:99:ARG:HD3	5:F:99:ARG:HA	1.76	0.45
5:F:572:THR:O	5:F:576:VAL:HG23	2.17	0.45
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	1.99	0.45
5:L:511:ILE:HD12	5:L:511:ILE:HA	1.84	0.45
2:C:488:MET:O	2:C:490:GLN:N	2.44	0.45
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.97	0.45
2:I:239:MET:O	2:I:284:LEU:HD12	2.16	0.45
3:J:839:VAL:HG13	3:J:882:VAL:HG21	1.98	0.45
1:B:101:THR:HA	1:B:142:MET:O	2.17	0.45
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.77	0.45
2:I:494:ASN:HB3	2:I:497:PRO:HD2	1.98	0.45
2:I:816:ILE:HG22	2:I:818:VAL:HG23	1.98	0.45
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.50	0.45
3:J:905:ARG:NH1	3:J:910:ASN:HD21	2.14	0.45
1:A:167:PRO:HB2	1:A:170:ARG:HG3	1.99	0.44
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.81	0.44
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.98	0.44
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.50	0.44
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.51	0.44
5:F:399:LEU:HD12	5:F:399:LEU:HA	1.79	0.44
1:G:154:PRO:HB2	2:I:1059:ARG:NH2	2.32	0.44
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:724:VAL:HA	2:I:734:ILE:HD13	1.98	0.44
3:J:334:LYS:HD2	3:J:334:LYS:HA	1.48	0.44
3:J:793:SER:O	3:J:797:THR:HG23	2.17	0.44
5:L:312:SER:OG	5:L:313:ASP:N	2.50	0.44
2:C:34:SER:HB2	2:C:455:SER:HB2	2.00	0.44
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.81	0.44
2:C:724:VAL:HG23	2:C:775:GLU:O	2.16	0.44
2:C:1116:HIS:CE1	3:D:641:ILE:HB	2.52	0.44
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.52	0.44
1:H:102:LEU:HD23	1:H:102:LEU:HA	1.82	0.44
2:I:462:ASN:O	2:I:465:ARG:HB3	2.17	0.44
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.82	0.44
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.80	0.44
3:D:749:LYS:HG3	3:D:753:SER:O	2.17	0.44
3:D:843:VAL:HG11	3:D:897:HIS:O	2.16	0.44
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.50	0.44
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.45	0.44
2:I:1247:SER:HB3	3:J:375:GLU:O	2.16	0.44
2:C:705:GLU:HB2	2:C:794:LEU:HB3	1.99	0.44
2:C:816:ILE:O	2:C:1076:ILE:HD12	2.18	0.44
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.83	0.44
3:D:751:ASP:OD2	3:D:753:SER:OG	2.36	0.44
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.52	0.44
5:F:575:GLU:O	5:F:579:GLN:HG2	2.18	0.44
1:H:133:LEU:HD12	1:H:133:LEU:HA	1.83	0.44
2:I:316:GLU:H	2:I:316:GLU:CD	2.21	0.44
2:I:864:LYS:NZ	2:I:876:GLU:O	2.51	0.44
2:C:1341:ASP:HB3	2:C:1342:GLU:H	1.43	0.44
3:D:31:ARG:NH2	3:D:106:GLU:OE2	2.42	0.44
3:D:548:VAL:HG12	3:D:550:VAL:HG13	2.00	0.44
1:H:102:LEU:HD12	1:H:142:MET:HG2	2.00	0.44
2:I:992:LEU:HD23	2:I:992:LEU:H	1.82	0.44
3:J:27:PRO:HD3	3:J:236:TRP:CD1	2.53	0.44
5:L:96:ASP:O	5:L:98:VAL:N	2.51	0.44
1:B:8:PHE:HD1	1:B:9:LEU:H	1.65	0.44
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.77	0.44
3:D:1227:HIS:CD2	3:J:1292:LEU:HB3	2.52	0.44
2:I:591:TYR:N	2:I:604:HIS:O	2.51	0.44
3:J:824:PRO:HD3	3:J:835:LEU:HD13	1.98	0.44
3:J:1290:ARG:HA	3:J:1290:ARG:HD3	1.83	0.44
5:L:547:VAL:HG22	5:L:603:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD23	1:B:79:LEU:H	1.82	0.44
1:B:109:PRO:HB3	1:B:132:HIS:HD2	1.81	0.44
3:D:122:SER:O	3:D:126:LEU:HG	2.16	0.44
5:F:577:GLY:HA2	5:F:587:ILE:HD11	2.00	0.44
1:G:70:THR:CG2	2:I:755:LYS:HE2	2.48	0.44
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.82	0.44
2:I:1307:ASN:HB3	2:I:1312:ASN:O	2.17	0.44
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.99	0.44
3:J:599:LYS:HA	3:J:599:LYS:HD3	1.77	0.44
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.99	0.44
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.99	0.44
3:J:45:ASN:HB3	3:J:48:THR:O	2.17	0.44
3:J:356:THR:OG1	3:J:357:VAL:N	2.42	0.44
3:J:520:ALA:HB1	3:J:543:SER:HB3	2.00	0.44
3:J:702:GLN:HB3	3:J:702:GLN:HE21	1.62	0.44
5:L:600:HIS:CD2	5:L:601:PRO:HD2	2.53	0.44
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.99	0.44
2:C:169:LYS:O	2:C:169:LYS:HG2	2.18	0.44
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	2.00	0.44
2:C:1308:ILE:HG23	3:D:380:PHE:CE2	2.53	0.44
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.98	0.44
1:H:101:THR:HA	1:H:142:MET:O	2.18	0.44
2:I:229:ILE:HB	2:I:240:GLU:HB2	1.98	0.44
5:L:585:GLU:O	5:L:589:GLN:HG3	2.18	0.44
2:C:462:ASN:O	2:C:465:ARG:HB3	2.18	0.43
3:D:45:ASN:HB3	3:D:48:THR:O	2.18	0.43
3:D:275:ARG:HD3	3:D:298:MET:HB3	2.00	0.43
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	1.98	0.43
5:F:600:HIS:CD2	5:F:601:PRO:HD2	2.53	0.43
1:G:207:THR:HG22	1:G:208:ASN:H	1.82	0.43
2:I:816:ILE:O	2:I:1076:ILE:HD12	2.18	0.43
3:J:397:ALA:O	3:J:401:VAL:HG13	2.18	0.43
3:J:557:LYS:HE3	3:J:557:LYS:HB2	1.79	0.43
3:J:827:GLU:C	3:J:829:GLY:H	2.20	0.43
3:J:858:VAL:HA	3:J:859:PRO:HD3	1.76	0.43
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.99	0.43
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.82	0.43
5:L:551:LEU:HD23	5:L:597:LYS:HD2	2.00	0.43
2:C:250:THR:HA	2:C:268:ARG:HA	2.00	0.43
2:C:582:ASN:OD1	2:C:583:GLU:N	2.51	0.43
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.18	0.43
3:D:27:PRO:HD3	3:D:236:TRP:CD1	2.53	0.43
3:D:814:CYS:HB3	3:D:890:THR:OG1	2.19	0.43
2:I:169:LYS:O	2:I:169:LYS:HG2	2.18	0.43
2:I:269:ILE:HG23	2:I:273:HIS:HB2	2.00	0.43
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.00	0.43
2:C:316:GLU:CD	2:C:316:GLU:H	2.21	0.43
2:C:591:TYR:N	2:C:604:HIS:O	2.50	0.43
3:D:931:THR:OG1	3:D:1244:GLN:NE2	2.52	0.43
5:F:105:MET:HB2	5:F:105:MET:HE2	1.44	0.43
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.19	0.43
3:D:262:THR:C	5:F:507:MET:HB2	2.38	0.43
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.79	0.43
3:D:647:PRO:HG3	3:D:697:MET:HB3	2.01	0.43
5:F:583:THR:HG22	5:F:584:ARG:H	1.83	0.43
2:I:127:ILE:HA	2:I:128:PRO:HD3	1.89	0.43
2:I:488:MET:O	2:I:490:GLN:N	2.44	0.43
3:J:94:GLN:O	3:J:97:VAL:HG23	2.19	0.43
3:J:527:LEU:HB2	3:J:550:VAL:HG12	2.00	0.43
3:J:702:GLN:HG2	3:J:703:THR:N	2.34	0.43
3:J:1022:PRO:HG2	3:J:1023:HIS:CD2	2.54	0.43
1:A:66:HIS:HD2	2:C:874:GLY:HA2	1.84	0.43
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.52	0.43
1:B:195:ARG:HB3	1:B:198:LEU:HD21	2.01	0.43
2:C:697:LYS:HA	2:C:795:ALA:HB2	2.00	0.43
3:D:832:LYS:HD3	3:D:1242:ARG:HH12	1.83	0.43
4:E:15:ASN:HB3	4:E:18:ASP:HB2	2.00	0.43
1:H:109:PRO:HA	1:H:132:HIS:HA	1.99	0.43
2:I:133:ASN:OD1	2:I:713:GLY:HA3	2.19	0.43
2:I:697:LYS:HA	2:I:795:ALA:HB2	2.00	0.43
3:J:1264:ALA:HA	3:J:1305:ASP:HB2	1.99	0.43
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.48	0.43
1:A:115:ILE:HG22	1:A:116:THR:H	1.83	0.43
1:B:66:HIS:O	1:B:78:ILE:HD12	2.19	0.43
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.43
3:D:405:GLU:O	3:D:408:VAL:HG22	2.19	0.43
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.52	0.43
1:G:167:PRO:HB2	1:G:170:ARG:HG3	2.00	0.43
1:H:11:PRO:HB3	1:H:30:PRO:O	2.19	0.43
1:H:79:LEU:HD23	1:H:79:LEU:H	1.83	0.43
2:I:14:ASP:N	2:I:1157:GLN:OE1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:887:VAL:HB	2:I:913:VAL:HG22	2.01	0.43
2:I:1164:PHE:O	2:I:1169:VAL:HG23	2.19	0.43
3:J:341:ASN:HB2	3:J:1352:ILE:HD13	2.01	0.43
3:J:647:PRO:HG3	3:J:697:MET:HB3	2.00	0.43
3:J:832:LYS:HD3	3:J:1242:ARG:HH12	1.83	0.43
5:L:577:GLY:HA2	5:L:587:ILE:HD11	2.01	0.43
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.53	0.43
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.68	0.43
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.88	0.43
5:F:551:LEU:HD23	5:F:597:LYS:HD2	1.99	0.43
2:I:69:GLN:NE2	2:I:101:ARG:HD2	2.33	0.43
2:I:144:VAL:HG23	2:I:515:MET:HB2	2.00	0.43
2:I:156:PHE:CZ	2:I:445:ILE:HG13	2.54	0.43
2:C:56:VAL:HG11	2:C:468:LEU:HB3	2.00	0.43
2:C:59:ILE:HD13	2:C:472:GLU:HA	2.01	0.43
2:C:221:LEU:HD11	2:C:314:ASN:CB	2.44	0.43
3:D:1227:HIS:CD2	3:J:1293:GLU:H	2.37	0.43
3:D:1346:GLY:O	3:D:1350:ASN:ND2	2.45	0.43
4:E:31:GLN:HE21	4:E:46:THR:HG21	1.84	0.43
2:I:1151:LEU:HD11	2:I:1198:LEU:HD23	2.01	0.43
3:J:733:SER:O	3:J:737:ILE:HG12	2.19	0.43
2:C:24:VAL:HG21	2:C:704:MET:SD	2.59	0.43
2:C:269:ILE:HG23	2:C:273:HIS:HB2	2.00	0.43
3:D:702:GLN:HG2	3:D:703:THR:N	2.34	0.43
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.84	0.43
5:F:96:ASP:O	5:F:98:VAL:N	2.52	0.43
1:H:71:LYS:HD2	1:H:71:LYS:HA	1.71	0.43
2:I:582:ASN:HB3	2:I:586:PHE:N	2.34	0.43
3:J:489:ASN:HA	3:J:904:ALA:HB1	2.00	0.43
3:J:770:LEU:O	3:J:774:ILE:HG13	2.19	0.43
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.33	0.43
2:C:144:VAL:HG23	2:C:515:MET:HB2	2.01	0.43
2:C:678:ARG:CZ	2:C:1106:ARG:HG2	2.49	0.43
2:C:799:ASN:HA	2:C:1231:TYR:HA	2.01	0.43
3:D:124:ILE:HG23	3:D:189:LEU:HD11	2.00	0.43
3:D:349:TYR:CE2	3:D:379:PRO:HG2	2.52	0.43
3:D:801:VAL:O	3:D:805:GLN:HB2	2.19	0.43
3:D:824:PRO:HD3	3:D:835:LEU:HD13	1.99	0.43
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.84	0.43
3:D:1137:GLY:O	3:D:1140:ARG:HB3	2.19	0.43
5:F:350:GLU:H	5:F:350:GLU:HG3	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:THR:HG22	1:G:208:ASN:N	2.34	0.43
1:H:33:ARG:NH1	2:I:1081:PRO:HG3	2.33	0.43
2:I:24:VAL:HG21	2:I:704:MET:SD	2.58	0.43
2:I:250:THR:HA	2:I:268:ARG:HA	2.00	0.43
2:I:930:ASP:OD2	2:I:931:VAL:N	2.51	0.43
2:I:1116:HIS:CE1	3:J:641:ILE:H	2.30	0.43
3:J:45:ASN:O	3:J:46:TYR:HD2	2.02	0.43
2:C:930:ASP:OD2	2:C:931:VAL:N	2.51	0.42
3:D:520:ALA:HB1	3:D:543:SER:HB3	2.01	0.42
3:D:901:ARG:HD2	3:D:906:GLY:O	2.19	0.42
4:E:45:LYS:O	4:E:49:ILE:HG13	2.19	0.42
5:F:311:THR:HG21	5:F:348:GLU:CD	2.40	0.42
1:H:34:GLY:HA3	2:I:1083:GLU:OE1	2.19	0.42
1:H:66:HIS:O	1:H:78:ILE:HD12	2.19	0.42
2:I:582:ASN:OD1	2:I:583:GLU:N	2.50	0.42
2:I:799:ASN:HA	2:I:1231:TYR:HA	2.01	0.42
3:J:814:CYS:HB3	3:J:890:THR:OG1	2.19	0.42
1:B:109:PRO:HA	1:B:132:HIS:HA	1.99	0.42
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.34	0.42
2:C:128:PRO:HG2	2:C:506:PHE:CD1	2.54	0.42
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.45	0.42
3:D:527:LEU:HB2	3:D:550:VAL:HG12	2.00	0.42
3:D:807:LEU:HD23	3:D:915:ILE:HG13	2.02	0.42
3:D:824:PRO:O	3:D:826:ILE:HG13	2.19	0.42
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.17	0.42
2:I:74:ARG:HH12	2:I:121:GLU:CD	2.22	0.42
2:I:356:THR:HG21	2:I:362:ALA:HA	2.02	0.42
2:I:867:GLU:H	2:I:867:GLU:HG3	1.62	0.42
3:J:77:ARG:HG3	3:J:79:LYS:H	1.84	0.42
3:J:611:ILE:HG22	3:J:612:LEU:HD12	2.01	0.42
3:J:751:ASP:OD2	3:J:753:SER:OG	2.36	0.42
3:J:1203:ARG:NH1	3:J:1205:GLU:HG2	2.33	0.42
2:C:55:SER:OG	2:C:56:VAL:N	2.52	0.42
2:C:452:ARG:NH1	2:C:585:GLY:HA3	2.34	0.42
2:C:669:PRO:O	2:C:1070:HIS:HE1	2.02	0.42
2:C:906:PHE:CE2	5:F:608:ARG:HG3	2.54	0.42
3:D:708:ASN:OD1	3:D:708:ASN:N	2.52	0.42
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.19	0.42
3:D:1348:LYS:O	3:D:1352:ILE:HG12	2.20	0.42
2:I:59:ILE:HD13	2:I:472:GLU:HA	2.02	0.42
3:J:124:ILE:HG23	3:J:189:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:325:LYS:HG3	3:J:329:ASP:HB2	2.01	0.42
3:J:931:THR:OG1	3:J:1244:GLN:NE2	2.52	0.42
1:A:48:LEU:HA	1:A:180:VAL:HG21	2.02	0.42
2:C:89:GLY:HA2	2:C:140:GLY:HA3	2.01	0.42
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.49	0.42
2:C:791:LEU:HD23	2:C:791:LEU:HA	1.80	0.42
2:C:1151:LEU:HD11	2:C:1198:LEU:HD23	2.01	0.42
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.02	0.42
3:D:94:GLN:O	3:D:97:VAL:HG23	2.20	0.42
3:D:615:LYS:HB2	3:D:616:PRO:HD3	2.01	0.42
3:D:646:ILE:HD11	3:D:764:ARG:HD2	2.01	0.42
3:D:709:ARG:HA	3:D:709:ARG:HD2	1.88	0.42
5:F:126:GLY:O	5:F:129:GLN:HB2	2.20	0.42
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.01	0.42
2:I:470:ARG:NE	2:I:497:PRO:HB3	2.33	0.42
2:I:1043:ALA:HB1	2:I:1044:PRO:HD2	2.01	0.42
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.01	0.42
3:J:901:ARG:HD2	3:J:906:GLY:O	2.19	0.42
3:D:487:THR:OG1	4:E:4:VAL:O	2.28	0.42
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.54	0.42
2:I:128:PRO:HG2	2:I:506:PHE:CD1	2.54	0.42
3:J:987:GLU:H	3:J:987:GLU:HG3	1.55	0.42
2:C:1164:PHE:O	2:C:1169:VAL:HG23	2.19	0.42
5:F:134:VAL:HG22	5:F:273:MET:HE3	2.02	0.42
1:H:91:ARG:H	1:H:91:ARG:HG2	1.69	0.42
2:I:23:ASP:OD1	2:I:23:ASP:N	2.52	0.42
2:I:55:SER:OG	2:I:56:VAL:N	2.52	0.42
2:I:1158:LYS:O	2:I:1159:VAL:HG13	2.20	0.42
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	2.02	0.42
3:J:646:ILE:HD11	3:J:764:ARG:HD2	2.01	0.42
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.18	0.42
2:C:349:GLU:O	2:C:353:VAL:HG23	2.19	0.42
2:C:887:VAL:HB	2:C:913:VAL:HG22	2.01	0.42
2:C:1136:GLN:HE21	2:C:1136:GLN:HB3	1.58	0.42
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.01	0.42
2:I:468:LEU:HD23	2:I:468:LEU:HA	1.92	0.42
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.54	0.42
2:I:678:ARG:CZ	2:I:1106:ARG:HG2	2.49	0.42
2:I:943:LYS:O	2:I:947:GLU:HG3	2.20	0.42
3:J:824:PRO:O	3:J:826:ILE:HG13	2.19	0.42
3:J:1344:LEU:O	3:J:1345:ARG:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:VAL:HG22	1:A:76:GLU:H	1.85	0.42
2:C:470:ARG:NE	2:C:497:PRO:HB3	2.34	0.42
2:C:739:ASP:OD1	2:C:739:ASP:N	2.53	0.42
2:C:867:GLU:H	2:C:867:GLU:HG3	1.62	0.42
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	2.02	0.42
2:C:1308:ILE:HG21	3:D:379:PRO:HB2	2.01	0.42
3:D:165:TYR:O	3:D:169:LEU:HB2	2.20	0.42
3:D:611:ILE:HG22	3:D:612:LEU:HD12	2.02	0.42
3:D:866:GLU:OE2	3:D:901:ARG:NH2	2.53	0.42
5:F:580:PHE:HD1	5:F:580:PHE:HA	1.70	0.42
1:H:215:GLU:HA	1:H:218:ARG:HD2	2.02	0.42
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.55	0.42
3:J:165:TYR:O	3:J:169:LEU:HB2	2.20	0.42
4:K:52:ARG:O	4:K:56:GLU:HG2	2.20	0.42
2:C:582:ASN:HB3	2:C:586:PHE:N	2.34	0.42
2:C:943:LYS:O	2:C:947:GLU:HG3	2.20	0.42
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.72	0.42
2:I:163:LYS:HB3	2:I:163:LYS:HE3	1.76	0.42
2:I:1297:ASP:OD1	2:I:1300:GLY:N	2.39	0.42
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.54	0.42
5:L:311:THR:HG21	5:L:348:GLU:CD	2.40	0.42
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.83	0.42
2:C:74:ARG:HH12	2:C:121:GLU:CD	2.22	0.42
3:D:77:ARG:HG3	3:D:79:LYS:H	1.84	0.42
3:D:325:LYS:HG3	3:D:329:ASP:HB2	2.02	0.42
3:D:361:LEU:HD22	3:D:365:GLN:HG3	2.01	0.42
3:D:368:LEU:HD22	3:D:373:ALA:HB2	2.02	0.42
3:D:907:HIS:HE1	4:E:11:GLU:OE2	2.03	0.42
3:D:1143:ASP:OD1	3:D:1148:ARG:NH1	2.53	0.42
3:D:1358:PRO:HB3	3:D:1366:HIS:CD2	2.55	0.42
2:I:349:GLU:O	2:I:353:VAL:HG23	2.19	0.42
3:J:156:ARG:NH2	3:J:191:SER:OG	2.53	0.42
3:J:405:GLU:O	3:J:408:VAL:HG22	2.19	0.42
3:J:548:VAL:HG12	3:J:550:VAL:HG13	2.01	0.42
1:B:11:PRO:HB3	1:B:30:PRO:O	2.20	0.41
2:C:468:LEU:HD23	2:C:468:LEU:HA	1.92	0.41
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.72	0.41
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.54	0.41
2:C:1086:PRO:O	2:C:1094:VAL:HG12	2.20	0.41
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.20	0.41
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1313:HIS:ND1	4:E:31:GLN:OE1	2.53	0.41
1:G:46:ILE:HD11	1:H:38:THR:HG21	2.02	0.41
2:I:801:ARG:HG2	2:I:1094:VAL:HG23	2.02	0.41
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	2.00	0.41
3:J:361:LEU:HD22	3:J:365:GLN:HG3	2.01	0.41
3:J:1348:LYS:O	3:J:1352:ILE:HG12	2.20	0.41
3:J:1355:ARG:NH1	3:J:1369:ARG:HH12	2.17	0.41
1:A:60:GLU:OE1	1:A:143:ARG:NH2	2.53	0.41
2:C:697:LYS:HB3	2:C:697:LYS:HE2	1.65	0.41
2:C:1304:MET:CE	3:D:472:LEU:HB3	2.50	0.41
3:D:1172:LYS:HA	3:D:1191:PRO:HA	2.02	0.41
5:F:161:LEU:HD12	5:F:161:LEU:HA	1.89	0.41
1:G:115:ILE:HG22	1:G:116:THR:H	1.84	0.41
2:I:183:TRP:HB2	2:I:199:ASP:HA	2.02	0.41
2:I:870:ILE:HG21	2:I:931:VAL:HG11	2.02	0.41
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.84	0.41
3:J:189:LEU:HB3	3:J:234:PRO:HB2	2.02	0.41
3:J:801:VAL:O	3:J:805:GLN:HB2	2.19	0.41
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	2.03	0.41
3:J:1347:LEU:HG	3:J:1357:ILE:HG23	2.02	0.41
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.82	0.41
2:C:566:GLY:O	2:C:569:ILE:HG13	2.20	0.41
2:C:715:THR:OG1	2:C:716:ALA:N	2.53	0.41
3:D:45:ASN:O	3:D:46:TYR:HD2	2.02	0.41
3:D:461:PHE:HD2	3:D:461:PHE:HA	1.74	0.41
5:F:583:THR:HG22	5:F:584:ARG:N	2.35	0.41
2:I:13:LYS:HZ1	2:I:1151:LEU:HB2	1.84	0.41
2:I:21:VAL:HG13	2:I:655:VAL:HG13	2.02	0.41
2:I:452:ARG:NH1	2:I:585:GLY:HA3	2.35	0.41
3:J:275:ARG:HD3	3:J:298:MET:HB3	2.01	0.41
3:J:878:ASP:OD2	3:J:991:THR:N	2.36	0.41
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.84	0.41
5:L:299:LYS:O	5:L:303:ILE:HG12	2.20	0.41
1:A:201:LEU:HG	1:A:203:ILE:HG13	2.03	0.41
1:A:207:THR:HG22	1:A:208:ASN:N	2.34	0.41
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	2.02	0.41
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.83	0.41
5:F:299:LYS:O	5:F:303:ILE:HG12	2.20	0.41
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	2.02	0.41
1:G:49:SER:OG	1:G:50:SER:N	2.53	0.41
1:G:60:GLU:OE1	1:G:143:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:566:GLY:O	2:I:569:ILE:HG13	2.21	0.41
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.49	0.41
3:J:709:ARG:O	3:J:711:GLY:N	2.51	0.41
3:J:918:ILE:HG13	3:J:919:ALA:N	2.31	0.41
5:L:126:GLY:O	5:L:130:VAL:HG13	2.20	0.41
5:L:515:GLU:HG2	5:L:516:ASP:N	2.35	0.41
2:C:356:THR:HG21	2:C:362:ALA:HA	2.02	0.41
2:C:1007:LYS:O	2:C:1011:LEU:HG	2.21	0.41
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	2.03	0.41
3:D:709:ARG:O	3:D:711:GLY:N	2.52	0.41
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.34	0.41
2:I:109:ALA:HB1	2:I:111:GLU:HA	2.02	0.41
3:J:349:TYR:CD1	3:J:472:LEU:HD11	2.55	0.41
3:J:363:LEU:O	3:J:363:LEU:HG	2.21	0.41
3:J:368:LEU:HD22	3:J:373:ALA:HB2	2.03	0.41
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.88	0.41
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.88	0.41
5:L:467:SER:O	5:L:471:LEU:HB2	2.21	0.41
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.70	0.41
5:L:601:PRO:HA	5:L:604:SER:H	1.86	0.41
2:C:23:ASP:OD1	2:C:23:ASP:N	2.52	0.41
2:C:519:ASN:HA	2:C:520:PRO:HD3	1.93	0.41
2:C:705:GLU:HB2	2:C:794:LEU:H	1.86	0.41
3:D:733:SER:O	3:D:737:ILE:HG12	2.20	0.41
1:G:90:VAL:HG22	1:G:91:ARG:H	1.86	0.41
1:G:190:ALA:H	1:G:199:ASP:HA	1.86	0.41
1:H:195:ARG:HB3	1:H:198:LEU:HD21	2.02	0.41
2:I:478:ARG:HH12	2:I:482:GLY:HA2	1.85	0.41
2:I:1288:GLN:HE21	3:J:1355:ARG:HA	1.85	0.41
3:J:799:ARG:NH1	3:J:1146:GLU:OE1	2.54	0.41
3:J:800:LEU:O	3:J:803:VAL:HG12	2.20	0.41
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.86	0.41
1:A:90:VAL:HG22	1:A:91:ARG:H	1.86	0.41
1:B:78:ILE:O	1:B:82:LEU:HG	2.21	0.41
2:C:138:ILE:HG22	2:C:139:ASN:N	2.35	0.41
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.85	0.41
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.56	0.41
3:D:1137:GLY:O	3:D:1141:VAL:HG23	2.21	0.41
5:F:281:ARG:O	5:F:285:ARG:HG3	2.21	0.41
5:F:467:SER:O	5:F:471:LEU:HB2	2.20	0.41
5:F:479:THR:OG1	5:F:480:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:ILE:O	1:H:82:LEU:HG	2.21	0.41
2:I:791:LEU:HD23	2:I:791:LEU:HA	1.81	0.41
2:I:976:ARG:HD2	2:I:989:LEU:HD23	2.02	0.41
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.32	0.41
2:C:53:PHE:O	2:C:57:PHE:HB2	2.21	0.41
2:C:870:ILE:HG21	2:C:931:VAL:HG11	2.02	0.41
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.86	0.41
2:C:976:ARG:HD2	2:C:989:LEU:HD23	2.02	0.41
3:D:827:GLU:C	3:D:829:GLY:H	2.21	0.41
3:D:1371:ARG:HH21	3:J:854:ALA:HA	1.85	0.41
4:E:8:ASP:HB2	4:E:55:GLU:HG2	2.03	0.41
2:I:715:THR:OG1	2:I:716:ALA:N	2.53	0.41
3:J:642:ASP:HA	3:J:764:ARG:NH2	2.36	0.41
2:C:13:LYS:NZ	2:C:1151:LEU:HB2	2.36	0.41
2:C:97:ARG:HB3	2:C:121:GLU:HB2	2.03	0.41
2:C:153:PRO:O	2:C:401:GLY:HA2	2.20	0.41
3:D:337:ARG:HG3	3:D:1325:PHE:O	2.20	0.41
3:D:770:LEU:O	3:D:774:ILE:HG13	2.21	0.41
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.33	0.41
4:E:39:VAL:HG22	4:E:40:PRO:HD2	2.03	0.41
1:H:178:SER:HA	1:H:179:PRO:HD3	1.91	0.41
2:I:13:LYS:NZ	2:I:1151:LEU:HB2	2.36	0.41
2:I:97:ARG:HB3	2:I:121:GLU:HB2	2.02	0.41
2:I:153:PRO:O	2:I:401:GLY:HA2	2.21	0.41
2:I:669:PRO:O	2:I:1070:HIS:HE1	2.03	0.41
3:J:79:LYS:HB2	5:L:569:THR:H	1.85	0.41
5:L:134:VAL:HG22	5:L:273:MET:HE3	2.02	0.41
1:B:215:GLU:HA	1:B:218:ARG:HD2	2.02	0.41
2:C:933:VAL:HG11	2:C:945:ALA:HB2	2.03	0.41
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	2.03	0.41
3:D:156:ARG:NH2	3:D:191:SER:OG	2.53	0.41
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.21	0.41
5:F:276:MET:O	5:F:280:VAL:HG23	2.21	0.41
5:F:311:THR:HG21	5:F:348:GLU:OE1	2.22	0.41
5:F:461:ASN:O	5:F:465:ARG:HG2	2.20	0.41
5:F:515:GLU:HG2	5:F:516:ASP:N	2.34	0.41
1:H:31:LEU:HD13	1:H:31:LEU:HA	1.94	0.41
2:I:102:LEU:HB2	2:I:489:PRO:HG3	2.02	0.41
2:I:217:THR:HG23	2:I:351:LEU:HD13	2.03	0.41
2:I:705:GLU:HB2	2:I:794:LEU:H	1.86	0.41
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:898:GLU:OE1	2:I:898:GLU:N	2.54	0.41
3:J:975:ILE:HD11	3:J:1003:LEU:HD11	2.03	0.41
5:L:458:GLU:O	5:L:462:LYS:HG3	2.21	0.41
1:A:190:ALA:H	1:A:199:ASP:HA	1.86	0.40
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.56	0.40
2:C:143:ARG:NH2	2:C:507:GLY:O	2.51	0.40
2:C:967:LEU:HG	2:C:1021:LEU:HD13	2.03	0.40
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.18	0.40
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.85	0.40
3:D:349:TYR:CD1	3:D:472:LEU:HD11	2.56	0.40
3:D:839:VAL:HG12	3:D:864:LEU:HD12	2.03	0.40
4:E:16:ARG:O	4:E:16:ARG:HG2	2.20	0.40
5:F:343:LYS:O	5:F:347:ILE:HG13	2.21	0.40
5:F:458:GLU:O	5:F:462:LYS:HG3	2.21	0.40
5:F:557:LYS:HB3	5:F:580:PHE:HZ	1.86	0.40
1:G:74:VAL:HG22	1:G:76:GLU:H	1.85	0.40
1:G:145:LYS:HE3	1:G:145:LYS:HB3	1.81	0.40
2:I:53:PHE:O	2:I:57:PHE:HB2	2.21	0.40
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.86	0.40
2:I:967:LEU:HG	2:I:1021:LEU:HD13	2.03	0.40
2:I:972:PHE:HD2	2:I:972:PHE:HA	1.79	0.40
3:J:79:LYS:HG3	3:J:80:HIS:N	2.36	0.40
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.37	0.40
3:J:596:LEU:HD12	3:J:601:ILE:HG13	2.03	0.40
3:J:839:VAL:HG12	3:J:864:LEU:HD12	2.03	0.40
5:L:557:LYS:HB3	5:L:580:PHE:HZ	1.86	0.40
1:A:49:SER:OG	1:A:50:SER:N	2.53	0.40
2:C:62:TYR:C	2:C:64:GLY:H	2.24	0.40
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	2.02	0.40
2:C:1111:GLN:O	2:C:1115:THR:OG1	2.35	0.40
3:D:596:LEU:HD12	3:D:601:ILE:HG13	2.03	0.40
3:D:642:ASP:HA	3:D:764:ARG:NH2	2.36	0.40
3:D:800:LEU:O	3:D:803:VAL:HG12	2.21	0.40
3:D:918:ILE:HG13	3:D:919:ALA:N	2.31	0.40
3:D:1344:LEU:O	3:D:1345:ARG:HB2	2.22	0.40
5:F:585:GLU:O	5:F:589:GLN:HG3	2.22	0.40
5:F:601:PRO:HA	5:F:604:SER:H	1.86	0.40
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.56	0.40
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.21	0.40
2:I:1007:LYS:O	2:I:1011:LEU:HG	2.20	0.40
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	2.03	0.40
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.56	0.40
3:J:77:ARG:HG3	3:J:79:LYS:HB3	2.03	0.40
3:J:646:ILE:H	3:J:646:ILE:HG12	1.59	0.40
3:J:701:LEU:CD1	3:J:723:TYR:HB2	2.52	0.40
3:J:988:PHE:HD2	3:J:990:ARG:HH21	1.67	0.40
3:J:1172:LYS:HA	3:J:1191:PRO:HA	2.02	0.40
5:L:276:MET:O	5:L:280:VAL:HG23	2.21	0.40
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.34	0.40
5:L:281:ARG:O	5:L:285:ARG:HG3	2.21	0.40
1:A:35:PHE:HD1	1:A:35:PHE:HA	1.76	0.40
1:A:145:LYS:HE3	1:A:145:LYS:HB3	1.81	0.40
2:C:453:ILE:HD11	2:C:530:ILE:HD12	2.02	0.40
3:D:298:MET:SD	5:F:402:LEU:HB3	2.61	0.40
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.03	0.40
1:G:231:PHE:CE1	1:H:221:ALA:HB3	2.55	0.40
1:H:109:PRO:HB3	1:H:132:HIS:CD2	2.56	0.40
2:I:1178:LYS:HA	2:I:1178:LYS:HD3	1.76	0.40
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.72	0.40
3:J:355:ILE:HG21	3:J:466:MET:HG3	2.04	0.40
3:J:708:ASN:OD1	3:J:708:ASN:N	2.52	0.40
3:J:1143:ASP:OD1	3:J:1148:ARG:NH1	2.53	0.40
2:C:127:ILE:HA	2:C:128:PRO:HD3	1.89	0.40
2:C:870:ILE:HB	2:C:944:ARG:HD3	2.03	0.40
2:C:924:VAL:HG12	2:C:1058:ARG:HH21	1.86	0.40
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	2.02	0.40
3:D:27:PRO:O	3:D:31:ARG:HG3	2.22	0.40
3:D:1227:HIS:HB2	3:J:1293:GLU:HA	2.04	0.40
3:D:1347:LEU:HG	3:D:1357:ILE:HG23	2.03	0.40
5:F:119:ILE:O	5:F:123:ILE:HG13	2.21	0.40
1:H:179:PRO:HA	1:H:208:ASN:ND2	2.36	0.40
2:I:1086:PRO:O	2:I:1094:VAL:HG12	2.21	0.40
2:I:1149:TYR:OH	2:I:1176:LEU:HD11	2.22	0.40
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	2.03	0.40
3:J:124:ILE:H	3:J:124:ILE:HG13	1.67	0.40
3:J:537:TYR:CZ	3:J:544:LEU:HD13	2.57	0.40
3:J:1017:VAL:HG23	3:J:1018:ALA:H	1.86	0.40
5:L:105:MET:HE2	5:L:105:MET:HB2	1.43	0.40
5:L:299:LYS:HA	5:L:302:PHE:HB3	2.02	0.40
1:A:38:THR:HG21	1:B:46:ILE:HG13	2.04	0.40
2:C:60:GLN:H	2:C:60:GLN:HG2	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.85	0.40
3:D:195:GLU:O	3:D:198:CYS:HB2	2.21	0.40
5:F:567:MET:HE3	5:F:571:TYR:HE2	1.87	0.40
1:G:19:VAL:HG11	1:G:23:HIS:CE1	2.56	0.40
1:G:231:PHE:CZ	1:H:221:ALA:HB3	2.56	0.40
2:I:478:ARG:CZ	2:I:487:LEU:HD13	2.52	0.40
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.85	0.40
3:J:461:PHE:HD2	3:J:461:PHE:HA	1.75	0.40
3:J:1137:GLY:O	3:J:1141:VAL:HG23	2.21	0.40
5:L:95:THR:OG1	5:L:96:ASP:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	222/239 (93%)	194 (87%)	26 (12%)	2 (1%)	17 54
1	B	216/239 (90%)	192 (89%)	24 (11%)	0	100 100
1	G	226/239 (95%)	196 (87%)	28 (12%)	2 (1%)	17 54
1	H	213/239 (89%)	190 (89%)	23 (11%)	0	100 100
2	C	1338/1342 (100%)	1231 (92%)	102 (8%)	5 (0%)	34 69
2	I	1338/1342 (100%)	1230 (92%)	103 (8%)	5 (0%)	34 69
3	D	1162/1407 (83%)	1077 (93%)	81 (7%)	4 (0%)	41 74
3	J	1230/1407 (87%)	1145 (93%)	81 (7%)	4 (0%)	41 74
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100 100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100 100
5	F	464/522 (89%)	429 (92%)	35 (8%)	0	100 100
5	L	463/522 (89%)	427 (92%)	36 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	7036/7680 (92%)	6467 (92%)	547 (8%)	22 (0%)	41 74

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1159	VAL
2	I	1159	VAL
2	C	170	VAL
2	I	170	VAL
3	J	340	GLN
1	A	167	PRO
2	C	697	LYS
1	G	167	PRO
2	I	697	LYS
3	J	710	ASP
2	C	63	SER
2	C	1186	VAL
3	D	10	ALA
3	D	710	ASP
2	I	63	SER
2	I	1186	VAL
3	D	831	VAL
3	J	831	VAL
1	A	14	VAL
1	G	14	VAL
3	D	1180	VAL
3	J	1180	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	191/206 (93%)	174 (91%)	17 (9%)	9 37
1	B	184/206 (89%)	165 (90%)	19 (10%)	7 31
1	G	191/206 (93%)	174 (91%)	17 (9%)	9 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	183/206 (89%)	165 (90%)	18 (10%)	8 33
2	C	1155/1157 (100%)	1043 (90%)	112 (10%)	8 33
2	I	1154/1157 (100%)	1040 (90%)	114 (10%)	8 32
3	D	975/1168 (84%)	874 (90%)	101 (10%)	7 30
3	J	1036/1168 (89%)	929 (90%)	107 (10%)	7 31
4	E	72/75 (96%)	66 (92%)	6 (8%)	11 40
4	K	67/75 (89%)	60 (90%)	7 (10%)	7 30
5	F	417/462 (90%)	377 (90%)	40 (10%)	8 34
5	L	418/462 (90%)	376 (90%)	42 (10%)	7 32
All	All	6043/6548 (92%)	5443 (90%)	600 (10%)	8 32

All (600) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	ARG
1	A	13	LEU
1	A	54	CYS
1	A	61	ILE
1	A	74	VAL
1	A	79	LEU
1	A	133	LEU
1	A	137	ASN
1	A	145	LYS
1	A	158	ARG
1	A	165	GLU
1	A	182	ARG
1	A	186	ASN
1	A	215	GLU
1	A	219	ARG
1	A	231	PHE
1	B	7	GLU
1	B	8	PHE
1	B	12	ARG
1	B	18	GLN
1	B	50	SER
1	B	60	GLU
1	B	64	VAL
1	B	65	LEU

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	79	LEU
1	B	105	SER
1	B	124	VAL
1	B	131	CYS
1	B	133	LEU
1	B	134	THR
1	B	148	ARG
1	B	176	CYS
1	B	183	ILE
1	B	186	ASN
2	C	4	SER
2	C	11	ILE
2	C	22	LEU
2	C	53	PHE
2	C	82	VAL
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	117	ILE
2	C	118	LYS
2	C	119	GLU
2	C	120	GLN
2	C	121	GLU
2	C	124	MET
2	C	131	THR
2	C	132	ASP
2	C	164	THR
2	C	167	SER
2	C	179	TYR
2	C	201	ARG
2	C	285	ILE
2	C	299	LYS
2	C	305	SER
2	C	306	THR
2	C	369	MET
2	C	377	THR
2	C	394	ARG
2	C	396	ASP
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP

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Mol	Chain	Res	Type
2	C	445	ILE
2	C	455	SER
2	C	471	VAL
2	C	481	LEU
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	492	MET
2	C	496	LYS
2	C	508	SER
2	C	516	ASP
2	C	517	GLN
2	C	518	ASN
2	C	529	ARG
2	C	530	ILE
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	554	HIS
2	C	601	ASP
2	C	604	HIS
2	C	609	ILE
2	C	615	VAL
2	C	623	LEU
2	C	624	ASP
2	C	630	VAL
2	C	633	LEU
2	C	637	ARG
2	C	639	LYS
2	C	672	GLU
2	C	692	THR
2	C	697	LYS
2	C	705	GLU
2	C	714	VAL
2	C	748	ILE
2	C	764	CYS
2	C	765	ILE
2	C	773	LEU
2	C	778	GLU
2	C	779	ARG
2	C	788	SER
2	C	791	LEU

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Mol	Chain	Res	Type
2	C	799	ASN
2	C	800	MET
2	C	814	ASP
2	C	817	LEU
2	C	826	ASP
2	C	857	VAL
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	946	LEU
2	C	951	MET
2	C	974	ARG
2	C	984	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1019	ASP
2	C	1040	ASP
2	C	1073	LYS
2	C	1082	ILE
2	C	1109	ILE
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1156	ARG
2	C	1159	VAL
2	C	1163	THR
2	C	1198	LEU
2	C	1207	SER
2	C	1210	ILE
2	C	1238	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1327	LEU
2	C	1331	ARG
2	C	1342	GLU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP

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Mol	Chain	Res	Type
3	D	20	ILE
3	D	46	TYR
3	D	54	ASP
3	D	79	LYS
3	D	95	THR
3	D	106	GLU
3	D	159	ILE
3	D	169	LEU
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	194	LEU
3	D	217	LEU
3	D	230	SER
3	D	252	LEU
3	D	256	ASP
3	D	292	VAL
3	D	299	LEU
3	D	312	ARG
3	D	324	LEU
3	D	334	LYS
3	D	337	ARG
3	D	363	LEU
3	D	374	LEU
3	D	474	LEU
3	D	490	ILE
3	D	507	VAL
3	D	510	LEU
3	D	514	THR
3	D	523	GLU
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG
3	D	567	THR
3	D	573	THR
3	D	594	GLN
3	D	610	ARG
3	D	622	ASP
3	D	641	ILE
3	D	646	ILE
3	D	660	GLU
3	D	661	VAL

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Mol	Chain	Res	Type
3	D	678	ARG
3	D	683	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	702	GLN
3	D	704	GLU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	731	ARG
3	D	740	LEU
3	D	749	LYS
3	D	753	SER
3	D	754	ILE
3	D	764	ARG
3	D	770	LEU
3	D	788	LEU
3	D	801	VAL
3	D	805	GLN
3	D	810	THR
3	D	817	HIS
3	D	844	THR
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	858	VAL
3	D	860	ARG
3	D	878	ASP
3	D	895	CYS
3	D	897	HIS
3	D	898	CYS
3	D	908	ILE
3	D	918	ILE
3	D	1155	ILE
3	D	1169	THR
3	D	1177	ILE

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Mol	Chain	Res	Type
3	D	1186	TYR
3	D	1221	LEU
3	D	1255	VAL
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1293	GLU
3	D	1298	VAL
3	D	1305	ASP
3	D	1333	THR
3	D	1343	GLU
4	E	3	ARG
4	E	5	THR
4	E	8	ASP
4	E	13	ILE
4	E	39	VAL
4	E	46	THR
5	F	98	VAL
5	F	100	MET
5	F	102	MET
5	F	105	MET
5	F	154	GLU
5	F	247	GLU
5	F	266	PHE
5	F	267	ASP
5	F	297	MET
5	F	306	PHE
5	F	310	GLU
5	F	341	LEU
5	F	395	THR
5	F	422	ARG
5	F	429	THR
5	F	445	ASP
5	F	448	ARG
5	F	449	THR
5	F	472	GLN
5	F	476	ARG
5	F	479	THR
5	F	483	LEU

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Mol	Chain	Res	Type
5	F	485	GLU
5	F	486	ARG
5	F	489	MET
5	F	491	GLU
5	F	492	ASP
5	F	527	THR
5	F	530	LEU
5	F	547	VAL
5	F	552	THR
5	F	558	VAL
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	573	LEU
5	F	580	PHE
5	F	603	ARG
5	F	604	SER
5	F	609	SER
1	G	9	LEU
1	G	12	ARG
1	G	13	LEU
1	G	54	CYS
1	G	61	ILE
1	G	74	VAL
1	G	79	LEU
1	G	133	LEU
1	G	137	ASN
1	G	145	LYS
1	G	158	ARG
1	G	165	GLU
1	G	182	ARG
1	G	186	ASN
1	G	215	GLU
1	G	219	ARG
1	G	231	PHE
1	H	12	ARG
1	H	18	GLN
1	H	50	SER
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN

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Mol	Chain	Res	Type
1	H	79	LEU
1	H	105	SER
1	H	124	VAL
1	H	131	CYS
1	H	133	LEU
1	H	134	THR
1	H	148	ARG
1	H	158	ARG
1	H	176	CYS
1	H	183	ILE
1	H	186	ASN
2	I	4	SER
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	53	PHE
2	I	82	VAL
2	I	91	THR
2	I	108	GLU
2	I	115	LYS
2	I	116	ASP
2	I	117	ILE
2	I	118	LYS
2	I	119	GLU
2	I	121	GLU
2	I	124	MET
2	I	131	THR
2	I	132	ASP
2	I	164	THR
2	I	167	SER
2	I	179	TYR
2	I	201	ARG
2	I	285	ILE
2	I	299	LYS
2	I	305	SER
2	I	306	THR
2	I	369	MET
2	I	377	THR
2	I	394	ARG
2	I	396	ASP
2	I	419	ILE
2	I	423	ASP

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Mol	Chain	Res	Type
2	I	434	ASP
2	I	445	ILE
2	I	446	ASP
2	I	455	SER
2	I	471	VAL
2	I	481	LEU
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	487	LEU
2	I	492	MET
2	I	496	LYS
2	I	508	SER
2	I	516	ASP
2	I	517	GLN
2	I	529	ARG
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	554	HIS
2	I	601	ASP
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL
2	I	623	LEU
2	I	624	ASP
2	I	630	VAL
2	I	633	LEU
2	I	637	ARG
2	I	639	LYS
2	I	672	GLU
2	I	692	THR
2	I	697	LYS
2	I	705	GLU
2	I	714	VAL
2	I	748	ILE
2	I	764	CYS
2	I	765	ILE
2	I	773	LEU
2	I	778	GLU
2	I	779	ARG

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Mol	Chain	Res	Type
2	I	788	SER
2	I	791	LEU
2	I	799	ASN
2	I	800	MET
2	I	814	ASP
2	I	817	LEU
2	I	826	ASP
2	I	857	VAL
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	946	LEU
2	I	951	MET
2	I	974	ARG
2	I	984	VAL
2	I	992	LEU
2	I	1002	LEU
2	I	1019	ASP
2	I	1040	ASP
2	I	1073	LYS
2	I	1082	ILE
2	I	1109	ILE
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1156	ARG
2	I	1159	VAL
2	I	1163	THR
2	I	1198	LEU
2	I	1207	SER
2	I	1210	ILE
2	I	1238	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1327	LEU
2	I	1331	ARG
2	I	1342	GLU
3	J	18	ASP

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Mol	Chain	Res	Type
3	J	20	ILE
3	J	46	TYR
3	J	54	ASP
3	J	79	LYS
3	J	95	THR
3	J	106	GLU
3	J	159	ILE
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	194	LEU
3	J	217	LEU
3	J	230	SER
3	J	252	LEU
3	J	256	ASP
3	J	292	VAL
3	J	299	LEU
3	J	312	ARG
3	J	324	LEU
3	J	334	LYS
3	J	337	ARG
3	J	363	LEU
3	J	374	LEU
3	J	474	LEU
3	J	490	ILE
3	J	507	VAL
3	J	510	LEU
3	J	514	THR
3	J	523	GLU
3	J	536	LEU
3	J	545	HIS
3	J	547	ARG
3	J	567	THR
3	J	573	THR
3	J	594	GLN
3	J	610	ARG
3	J	622	ASP
3	J	641	ILE
3	J	646	ILE
3	J	660	GLU
3	J	661	VAL

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Mol	Chain	Res	Type
3	J	678	ARG
3	J	683	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	702	GLN
3	J	704	GLU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
3	J	712	GLN
3	J	717	VAL
3	J	720	ASN
3	J	731	ARG
3	J	740	LEU
3	J	749	LYS
3	J	753	SER
3	J	754	ILE
3	J	764	ARG
3	J	770	LEU
3	J	788	LEU
3	J	801	VAL
3	J	805	GLN
3	J	810	THR
3	J	817	HIS
3	J	844	THR
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	858	VAL
3	J	860	ARG
3	J	878	ASP
3	J	897	HIS
3	J	898	CYS
3	J	908	ILE
3	J	918	ILE
3	J	957	SER
3	J	960	LEU
3	J	963	VAL
3	J	972	LYS

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Mol	Chain	Res	Type
3	J	987	GLU
3	J	1011	VAL
3	J	1017	VAL
3	J	1027	VAL
3	J	1155	ILE
3	J	1163	VAL
3	J	1169	THR
3	J	1177	ILE
3	J	1186	TYR
3	J	1221	LEU
3	J	1255	VAL
3	J	1274	PHE
3	J	1275	LEU
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1293	GLU
3	J	1298	VAL
3	J	1305	ASP
3	J	1333	THR
3	J	1343	GLU
4	K	3	ARG
4	K	5	THR
4	K	13	ILE
4	K	28	ARG
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	98	VAL
5	L	100	MET
5	L	102	MET
5	L	105	MET
5	L	154	GLU
5	L	247	GLU
5	L	266	PHE
5	L	267	ASP
5	L	297	MET
5	L	306	PHE
5	L	310	GLU
5	L	341	LEU
5	L	395	THR

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Mol	Chain	Res	Type
5	L	422	ARG
5	L	429	THR
5	L	445	ASP
5	L	448	ARG
5	L	449	THR
5	L	472	GLN
5	L	476	ARG
5	L	479	THR
5	L	483	LEU
5	L	485	GLU
5	L	486	ARG
5	L	489	MET
5	L	491	GLU
5	L	492	ASP
5	L	527	THR
5	L	530	LEU
5	L	547	VAL
5	L	552	THR
5	L	558	VAL
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	573	LEU
5	L	574	GLU
5	L	580	PHE
5	L	603	ARG
5	L	604	SER
5	L	609	SER
5	L	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	132	HIS
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	573	ASN
2	C	620	ASN
2	C	628	HIS
2	C	1116	HIS
2	C	1134	GLN

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Mol	Chain	Res	Type
2	C	1136	GLN
2	C	1146	GLN
2	C	1288	GLN
3	D	200	GLN
3	D	266	ASN
3	D	702	GLN
3	D	792	ASN
3	D	861	ASN
3	D	907	HIS
3	D	910	ASN
3	D	929	GLN
3	D	1218	HIS
3	D	1227	HIS
3	D	1244	GLN
5	F	131	GLN
5	F	345	GLN
5	F	362	ASN
5	F	383	ASN
5	F	406	GLN
5	F	518	HIS
5	F	600	HIS
1	H	132	HIS
2	I	69	GLN
2	I	139	ASN
2	I	573	ASN
2	I	620	ASN
2	I	628	HIS
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1288	GLN
3	J	200	GLN
3	J	206	ASN
3	J	266	ASN
3	J	365	GLN
3	J	702	GLN
3	J	792	ASN
3	J	861	ASN
3	J	907	HIS
3	J	910	ASN
3	J	929	GLN

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Mol	Chain	Res	Type
3	J	979	ASN
3	J	1010	GLN
3	J	1023	HIS
3	J	1218	HIS
3	J	1244	GLN
5	L	131	GLN
5	L	345	GLN
5	L	362	ASN
5	L	383	ASN
5	L	406	GLN
5	L	518	HIS
5	L	600	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	42U	I	1401	-	31,34,34	1.40	7 (22%)	41,48,48	2.92	20 (48%)
6	42U	C	1401	-	31,34,34	1.42	7 (22%)	41,48,48	2.88	19 (46%)

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	42U	I	1401	-	-	7/20/28/28	1/4/4/4
6	42U	C	1401	-	-	7/20/28/28	1/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	42U	C13-C23	3.10	1.43	1.40
6	I	1401	42U	C13-C23	2.90	1.43	1.40
6	C	1401	42U	C25-C23	2.57	1.56	1.50
6	I	1401	42U	C25-C23	2.51	1.55	1.50
6	I	1401	42U	C12-C13	2.40	1.43	1.39
6	I	1401	42U	C16-N17	2.26	1.52	1.47
6	C	1401	42U	C18-C19	2.21	1.56	1.51
6	I	1401	42U	C16-C15	2.18	1.58	1.51
6	C	1401	42U	C12-C13	2.16	1.43	1.39
6	C	1401	42U	C15-N14	2.16	1.50	1.45
6	I	1401	42U	C18-C19	2.10	1.56	1.51
6	C	1401	42U	C16-C15	2.09	1.57	1.51
6	I	1401	42U	C15-N14	2.07	1.50	1.45
6	C	1401	42U	C16-N17	2.06	1.52	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	1401	42U	C12-C13-C23	-9.18	110.85	119.88
6	C	1401	42U	C12-C13-C23	-8.95	111.08	119.88
6	I	1401	42U	C04-C05-C08	6.53	130.96	120.61
6	C	1401	42U	C04-C05-C08	6.42	130.78	120.61
6	I	1401	42U	C05-C08-N31	-5.50	111.37	120.78
6	C	1401	42U	C05-C08-N31	-5.45	111.44	120.78
6	I	1401	42U	C11-C10-C24	-5.27	110.71	118.16
6	C	1401	42U	C11-C10-C24	-5.22	110.79	118.16
6	C	1401	42U	C21-C22-N17	4.63	117.59	110.94
6	I	1401	42U	C21-C22-N17	4.57	117.50	110.94
6	C	1401	42U	C11-C10-C09	4.44	128.10	120.91
6	I	1401	42U	C11-C10-C09	4.36	127.98	120.91
6	C	1401	42U	C07-C01-C03	-3.82	117.75	122.83
6	I	1401	42U	C07-C01-C03	-3.74	117.86	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1401	42U	C15-N14-C13	3.20	131.10	123.39
6	I	1401	42U	C15-N14-C13	3.19	131.06	123.39
6	I	1401	42U	C06-C05-C08	-3.14	115.64	120.61
6	I	1401	42U	C25-C23-C13	-3.10	118.44	120.72
6	C	1401	42U	C06-C05-C08	-3.06	115.76	120.61
6	I	1401	42U	C24-C23-C13	3.06	122.57	118.72
6	C	1401	42U	C25-C23-C13	-2.95	118.55	120.72
6	C	1401	42U	C24-C23-C13	2.95	122.44	118.72
6	I	1401	42U	C12-C11-C10	2.91	125.32	121.13
6	C	1401	42U	C12-C11-C10	2.85	125.24	121.13
6	C	1401	42U	C19-C18-N17	2.61	114.69	110.94
6	I	1401	42U	C19-C18-N17	2.52	114.55	110.94
6	C	1401	42U	C11-C12-C13	2.44	124.37	119.64
6	I	1401	42U	C11-C12-C13	2.43	124.33	119.64
6	C	1401	42U	C07-C06-C05	2.32	124.48	121.13
6	I	1401	42U	C07-C06-C05	2.25	124.38	121.13
6	I	1401	42U	C16-C15-N14	2.24	116.97	110.30
6	I	1401	42U	C03-C04-C05	2.24	124.36	121.13
6	C	1401	42U	C16-C15-N14	2.18	116.78	110.30
6	C	1401	42U	C03-C04-C05	2.16	124.25	121.13
6	I	1401	42U	C10-C24-C23	2.11	126.22	121.51
6	I	1401	42U	C06-C05-C04	-2.10	113.41	117.59
6	C	1401	42U	C06-C05-C04	-2.07	113.46	117.59
6	C	1401	42U	C10-C24-C23	2.05	126.09	121.51
6	I	1401	42U	F27-C25-C23	2.01	116.19	112.70

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1401	42U	N14-C15-C16-N17
6	I	1401	42U	N14-C15-C16-N17
6	C	1401	42U	C13-C23-C25-F27
6	I	1401	42U	C13-C23-C25-F27
6	C	1401	42U	C13-C23-C25-F28
6	I	1401	42U	C13-C23-C25-F28
6	C	1401	42U	C13-C23-C25-F26
6	I	1401	42U	C13-C23-C25-F26
6	C	1401	42U	C24-C23-C25-F27
6	I	1401	42U	C24-C23-C25-F27
6	C	1401	42U	C24-C23-C25-F28
6	I	1401	42U	C24-C23-C25-F28

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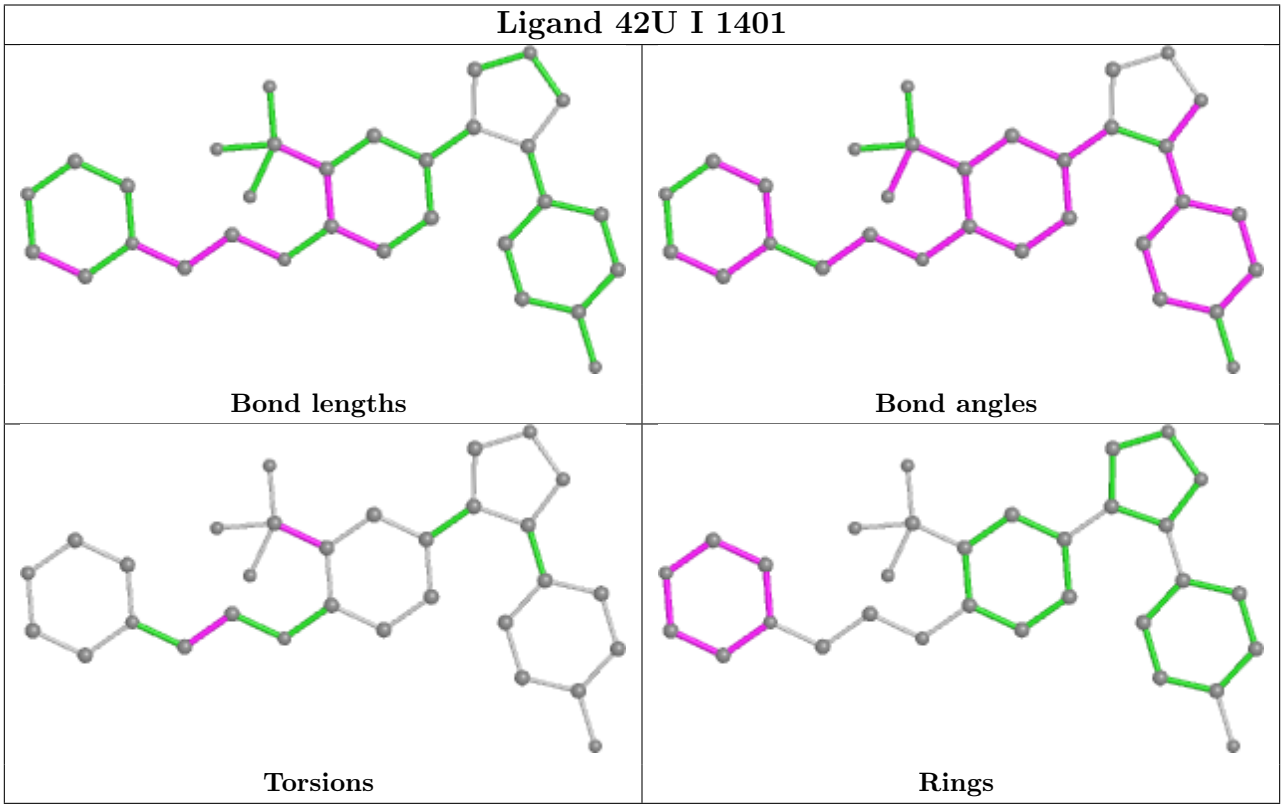
Mol	Chain	Res	Type	Atoms
6	C	1401	42U	C24-C23-C25-F26
6	I	1401	42U	C24-C23-C25-F26

All (2) ring outliers are listed below:

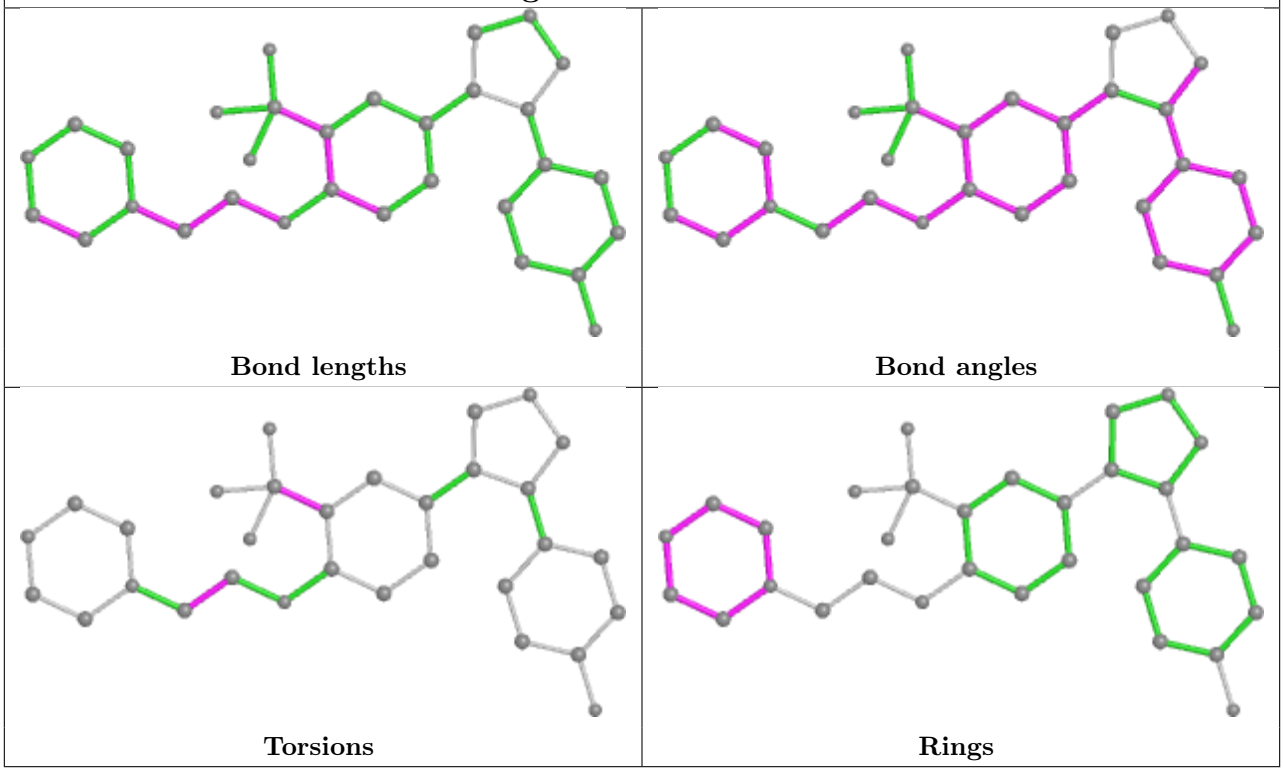
Mol	Chain	Res	Type	Atoms
6	C	1401	42U	C18-C19-C21-C22-N17-N20
6	I	1401	42U	C18-C19-C21-C22-N17-N20

No monomer is involved in short contacts.

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 then 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.



Ligand 42U C 1401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	224/239 (93%)	-0.18	4 (1%) 68 56	54, 87, 128, 162	0
1	B	220/239 (92%)	0.06	9 (4%) 37 26	71, 115, 149, 168	0
1	G	228/239 (95%)	-0.03	7 (3%) 49 35	74, 113, 149, 176	0
1	H	217/239 (90%)	0.23	16 (7%) 14 10	73, 129, 157, 174	0
2	C	1340/1342 (99%)	-0.20	18 (1%) 77 66	29, 79, 134, 171	0
2	I	1340/1342 (99%)	-0.11	27 (2%) 65 52	32, 96, 144, 171	0
3	D	1166/1407 (82%)	-0.13	25 (2%) 63 50	24, 78, 144, 177	0
3	J	1236/1407 (87%)	-0.04	34 (2%) 53 39	33, 95, 148, 172	0
4	E	89/91 (97%)	-0.37	0 100 100	40, 86, 123, 133	0
4	K	79/91 (86%)	-0.27	0 100 100	60, 92, 142, 160	0
5	F	470/522 (90%)	-0.02	27 (5%) 23 16	45, 121, 158, 182	0
5	L	469/522 (89%)	-0.13	24 (5%) 28 19	49, 117, 159, 180	0
All	All	7078/7680 (92%)	-0.10	191 (2%) 54 41	24, 96, 149, 182	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	160	HIS	6.5
3	D	1204	VAL	6.2
1	H	146	VAL	6.0
3	D	1198	VAL	5.4
5	F	167	ASP	5.3
3	D	878	ASP	5.2
2	C	982	GLY	5.0
3	J	1198	VAL	4.9
5	L	290	LEU	4.9
3	J	998	PRO	4.8
2	I	979	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
2	C	1000	LEU	4.7
5	L	305	LEU	4.7
3	D	858	VAL	4.7
3	J	1186	TYR	4.5
3	J	1161	GLY	4.4
3	D	879	ALA	4.4
3	D	857	LEU	4.3
2	I	1002	LEU	4.3
5	F	301	ASN	4.2
3	J	1294	ALA	4.2
5	F	92	GLY	4.1
1	B	65	LEU	3.8
5	F	579	GLN	3.8
5	F	300	LYS	3.7
1	H	58	GLU	3.7
5	F	283	GLN	3.6
5	L	317	ASN	3.6
3	D	1201	GLY	3.6
3	D	335	GLN	3.6
2	I	882	ILE	3.5
5	L	314	THR	3.5
1	H	98	VAL	3.5
3	J	859	PRO	3.4
2	I	995	ASP	3.4
5	F	476	ARG	3.4
3	J	1374	ALA	3.4
5	L	291	CYS	3.4
5	F	321	ALA	3.4
3	J	930	LEU	3.3
3	J	991	THR	3.3
5	L	315	TRP	3.3
3	J	1188	GLU	3.3
3	D	849	LEU	3.3
1	G	200	LYS	3.3
3	D	1199	PHE	3.3
2	I	1010	GLN	3.3
3	J	522	GLY	3.3
3	J	975	ILE	3.2
5	L	318	ALA	3.2
2	I	1003	THR	3.2
5	F	289	LYS	3.2
3	J	830	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	C	266	GLY	3.1
5	L	167	ASP	3.1
1	H	59	VAL	3.1
2	I	489	PRO	3.1
1	H	97	GLU	3.1
2	C	251	ALA	3.1
3	J	670	SER	3.1
3	J	683	ILE	3.0
2	C	252	SER	3.0
5	F	607	LEU	3.0
5	L	319	ALA	3.0
5	L	304	THR	3.0
1	G	211	ILE	3.0
5	F	290	LEU	3.0
2	C	282	VAL	2.9
3	D	1190	ILE	2.9
2	I	982	GLY	2.9
3	J	1028	ILE	2.9
5	F	581	ASP	2.9
1	H	57	THR	2.9
5	F	287	ILE	2.9
5	L	287	ILE	2.9
3	D	1210	ILE	2.9
2	I	1008	GLN	2.9
2	I	996	ARG	2.9
2	C	998	LEU	2.9
2	I	21	VAL	2.8
3	J	318	GLY	2.8
1	B	67	GLU	2.8
5	F	285	ARG	2.8
5	F	165	PHE	2.8
2	C	250	THR	2.8
5	L	261	LEU	2.8
1	B	13	LEU	2.7
2	C	1001	GLY	2.7
2	C	999	GLU	2.6
3	J	77	ARG	2.6
5	F	259	PHE	2.6
1	H	127	GLN	2.6
2	I	720	ARG	2.6
2	I	124	MET	2.6
3	D	859	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	I	989	LEU	2.6
2	I	251	ALA	2.6
2	I	6	THR	2.5
2	C	317	LEU	2.5
3	J	958	ILE	2.5
1	B	66	HIS	2.5
5	L	289	LYS	2.5
5	L	293	GLU	2.5
1	B	59	VAL	2.5
3	J	956	GLY	2.5
3	D	1173	ARG	2.5
3	D	880	VAL	2.4
3	J	1181	ASP	2.4
2	I	987	GLU	2.4
3	D	1287	ILE	2.4
1	H	122	GLU	2.4
5	L	294	GLN	2.4
3	J	768	ASN	2.4
2	I	420	LEU	2.4
3	D	856	ILE	2.4
3	J	1187	GLU	2.4
2	C	1002	LEU	2.4
3	J	999	TYR	2.4
3	J	1190	ILE	2.4
1	A	95	LYS	2.4
1	G	194	GLN	2.3
2	I	1211	ARG	2.3
5	L	300	LYS	2.3
1	H	49	SER	2.3
2	I	1001	GLY	2.3
5	F	158	LEU	2.3
5	F	340	ALA	2.3
3	D	756	GLU	2.3
1	H	91	ARG	2.3
3	D	1169	THR	2.3
3	D	1175	LEU	2.3
1	H	172	LEU	2.3
1	B	98	VAL	2.3
2	C	893	THR	2.3
5	F	474	MET	2.3
3	J	317	THR	2.3
1	G	123	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	267	ARG	2.2
5	F	603	ARG	2.2
3	D	1172	LYS	2.2
5	F	297	MET	2.2
5	F	554	ARG	2.2
5	L	480	PRO	2.2
3	J	959	LYS	2.2
3	D	1168	GLU	2.2
3	J	209	ASN	2.2
3	D	213	LYS	2.2
1	G	184	ALA	2.2
1	B	64	VAL	2.2
3	J	856	ILE	2.2
3	J	1369	ARG	2.2
5	F	286	LEU	2.2
1	A	194	GLN	2.2
2	C	964	LEU	2.2
1	A	221	ALA	2.2
3	J	972	LYS	2.2
3	J	1295	ASN	2.1
1	H	147	GLN	2.1
3	D	1171	GLY	2.1
5	F	293	GLU	2.1
5	F	111	LEU	2.1
5	L	307	THR	2.1
2	I	1014	LEU	2.1
5	L	165	PHE	2.1
5	L	610	PHE	2.1
5	L	313	ASP	2.1
5	F	580	PHE	2.1
3	J	973	LEU	2.1
1	G	25	LYS	2.1
1	A	98	VAL	2.1
2	I	978	VAL	2.1
2	I	492	MET	2.1
2	I	975	ILE	2.1
2	C	905	ILE	2.1
5	L	286	LEU	2.1
5	L	598	LEU	2.1
3	D	848	VAL	2.1
1	H	171	LEU	2.1
2	C	1215	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	I	247	ARG	2.0
3	J	1268	ASN	2.0
1	H	61	ILE	2.0
1	H	145	LYS	2.0
2	C	281	ASP	2.0
5	L	580	PHE	2.0
2	I	1004	ASP	2.0
5	F	591	GLU	2.0
1	H	20	SER	2.0
1	G	98	VAL	2.0
2	C	100	LEU	2.0
1	B	205	MET	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

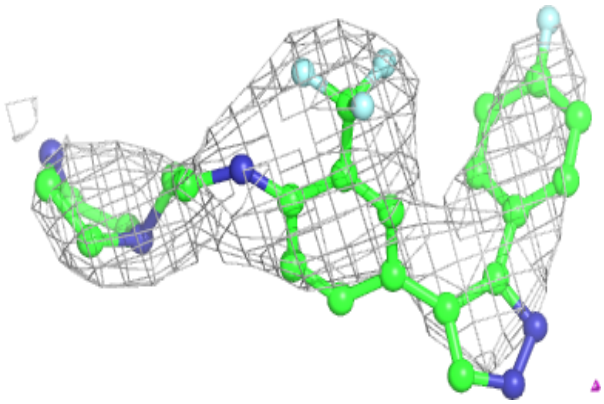
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	J	1501	1/1	0.84	0.61	75,75,75,75	0
6	42U	C	1401	31/31	0.89	0.33	31,71,93,105	0
6	42U	I	1401	31/31	0.91	0.33	48,83,117,134	0
7	MG	D	1501	1/1	0.93	0.36	42,42,42,42	0
8	ZN	J	1502	1/1	0.93	0.16	160,160,160,160	0
8	ZN	D	1503	1/1	0.94	0.25	76,76,76,76	0
8	ZN	D	1502	1/1	0.96	0.17	176,176,176,176	0
8	ZN	J	1503	1/1	0.98	0.27	126,126,126,126	0

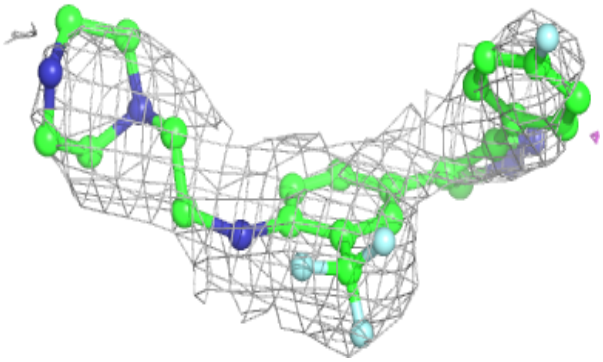
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

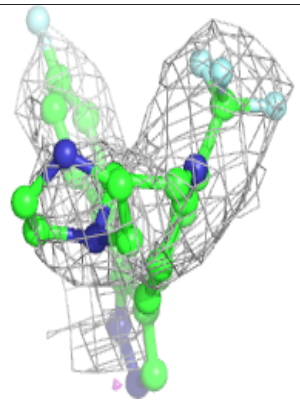
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 42U C 1401:

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

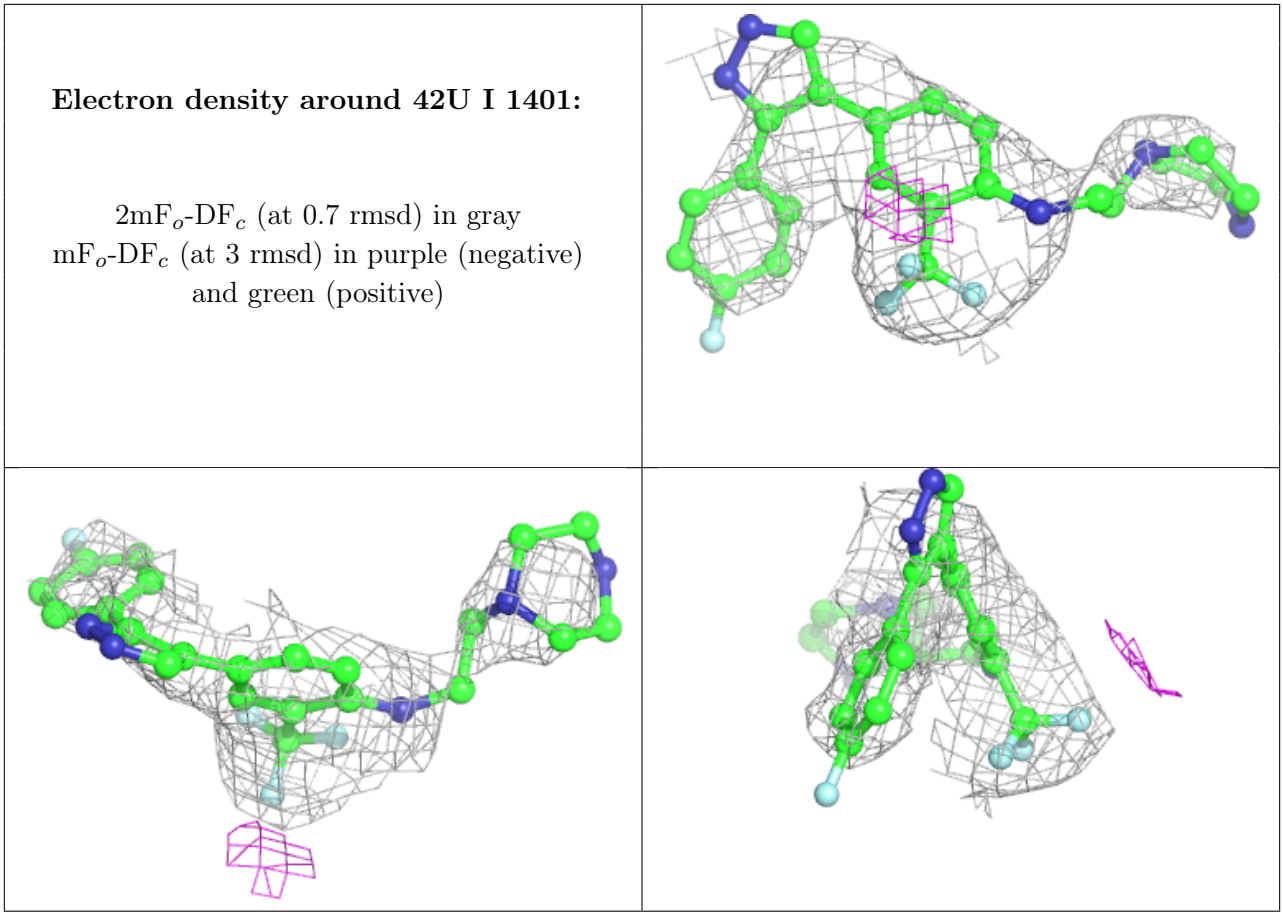






Electron density around 42U I 1401:

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



6.5 Other polymers

There are no such residues in this entry.