Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 03:58 AM EST

PDB ID	:	1YNJ
Title	:	Taq RNA polymerase-Sorangicin complex
Authors	:	Campbell, E.A.; Pavlova, O.; Zenkin, N.; Leon, F.; Irschik, H.; Jansen, R.; Severinov, K.; Darst, S.A.
Deposited on	:	2005-01-24
Resolution	:	3.20 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:

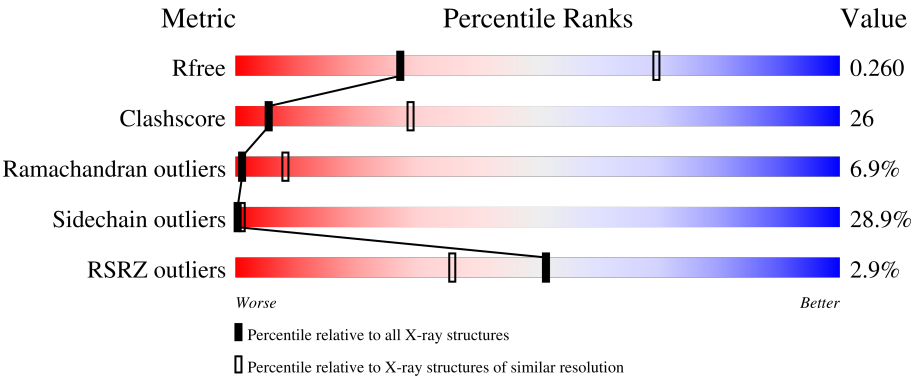
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	314	25% 32% 13% 27%
1	B	314	32% 30% 8% 28%
2	C	1119	39% 42% 15%
3	D	1524	4% 36% 33% 11% 19%
3	J	1524	7% 7% 84%

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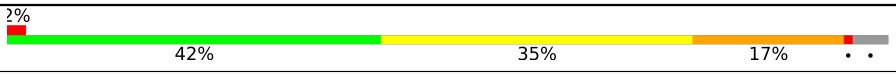
Mol	Chain	Length	Quality of chain
4	K	99	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 24369 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1763	1126	300	334	3			
1	B	225	Total	C	N	O	S	0	0	0
			1750	1118	300	329	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1114	Total	C	N	O	S	0	0	0
			8578	5431	1516	1607	24			

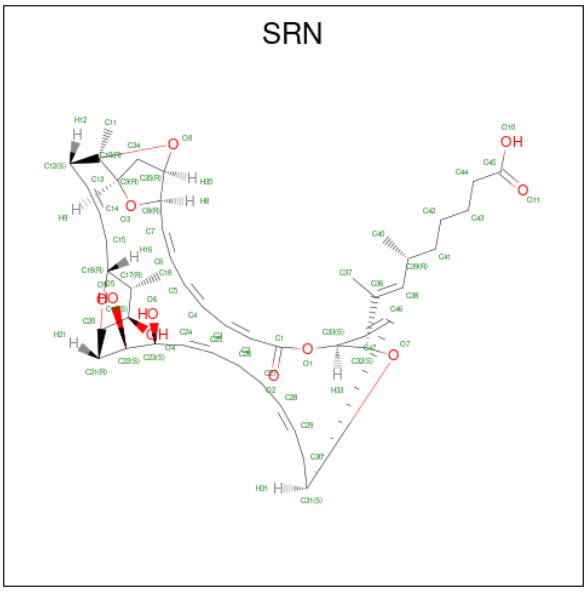
- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1238	Total	C	N	O	S	0	0	0
			9602	6065	1703	1798	36			
3	J	249	Total	C	N	O	S	0	0	0
			1869	1191	320	356	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	95	Total	C	N	O	S	0	0	0
			747	476	134	132	5			

- Molecule 5 is SORANGICIN A (three-letter code: SRN) (formula: $C_{47}H_{66}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 58 47 11	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

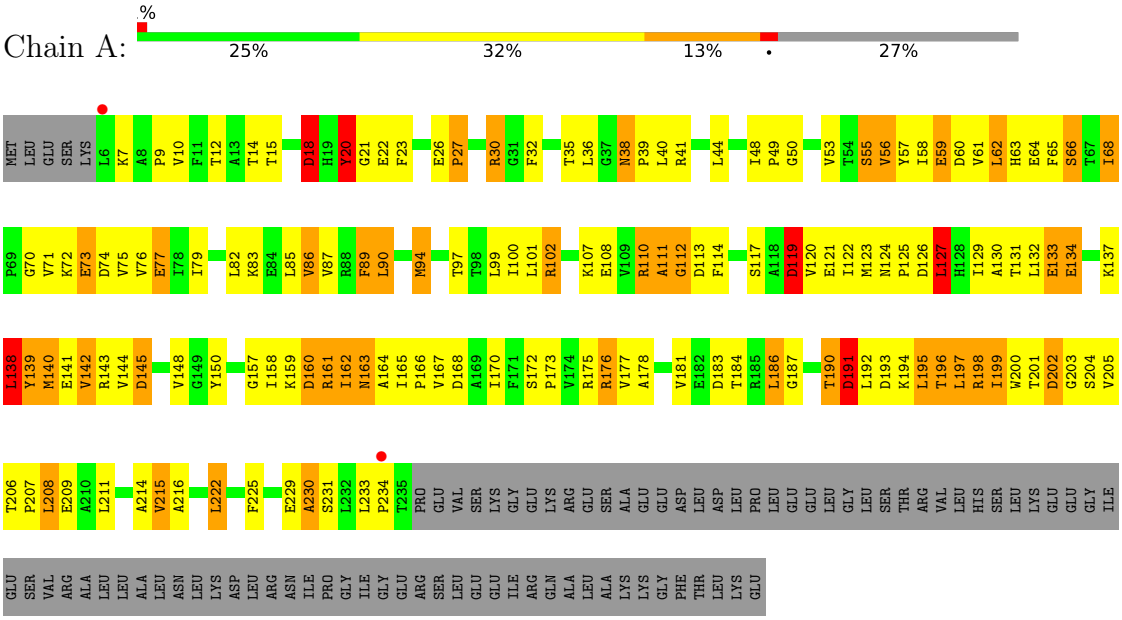
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	2	Total Zn 2 2	0	0

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.

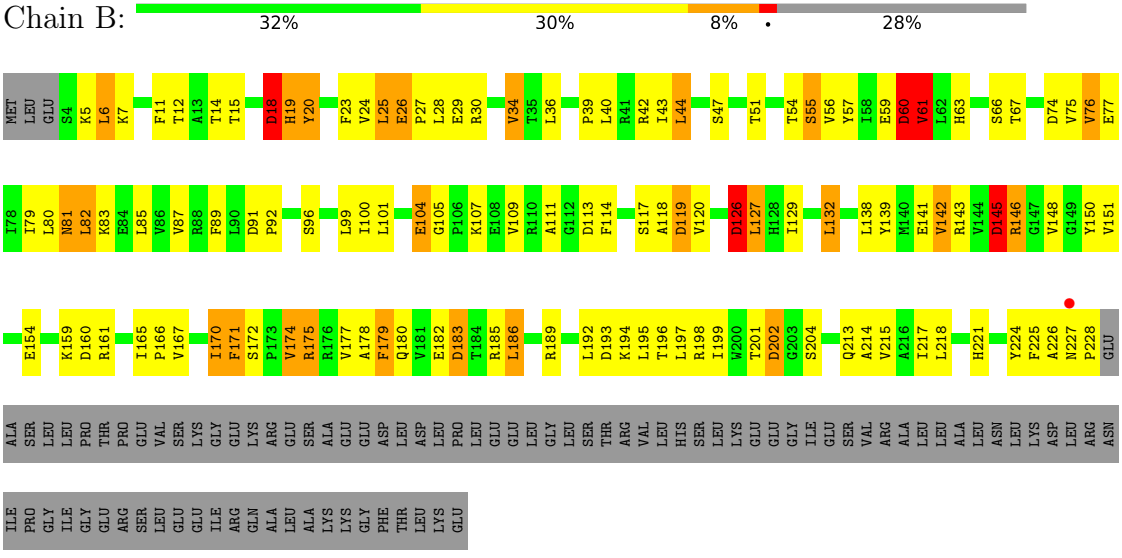
• Molecule 1: DNA-directed RNA polymerase alpha chain

Chain A:



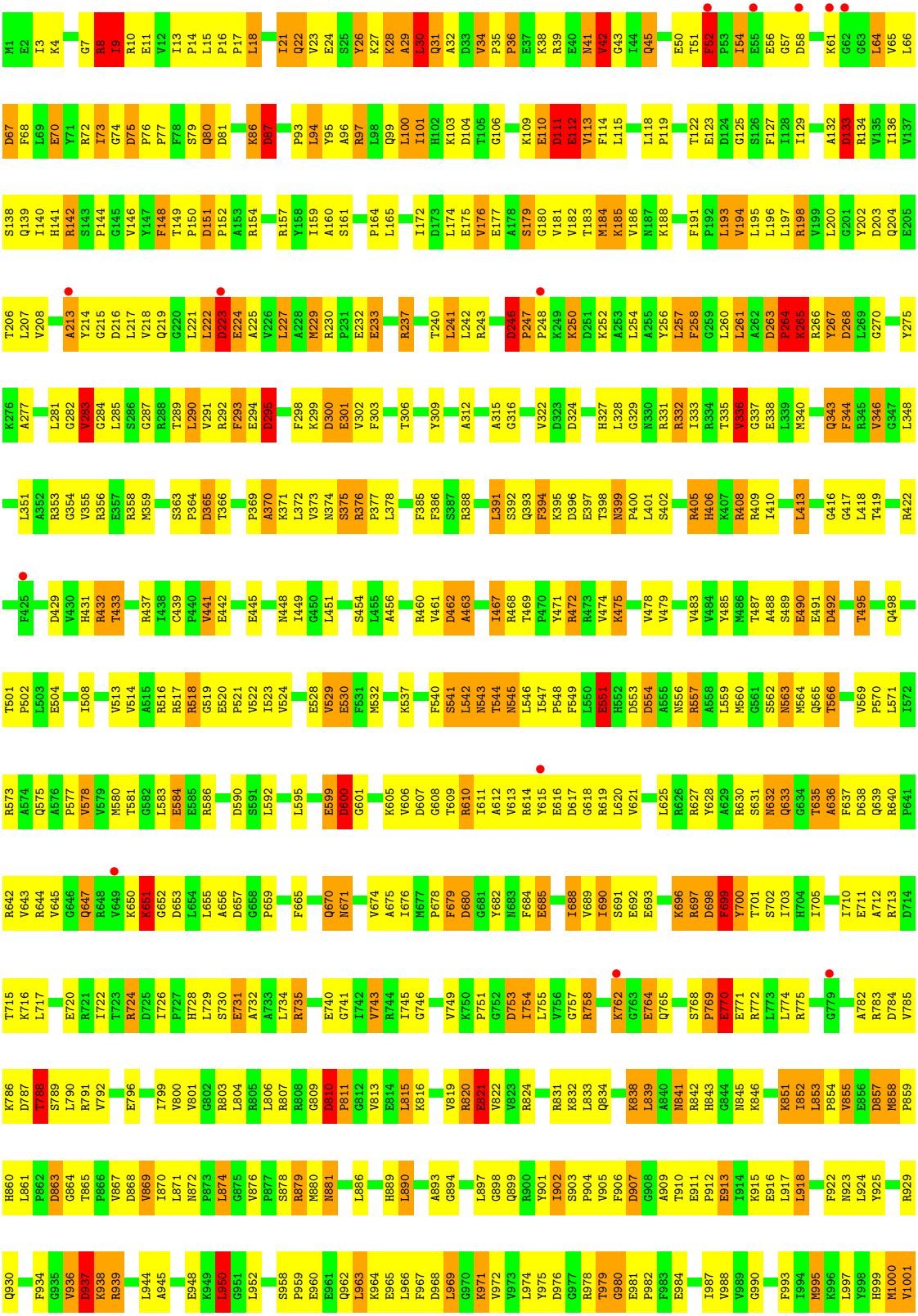
• Molecule 1: DNA-directed RNA polymerase alpha chain

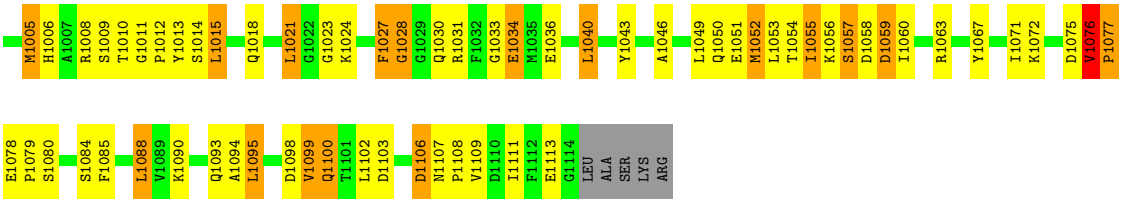
Chain B:



• Molecule 2: DNA-directed RNA polymerase beta chain

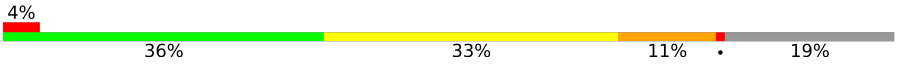
Chain C:

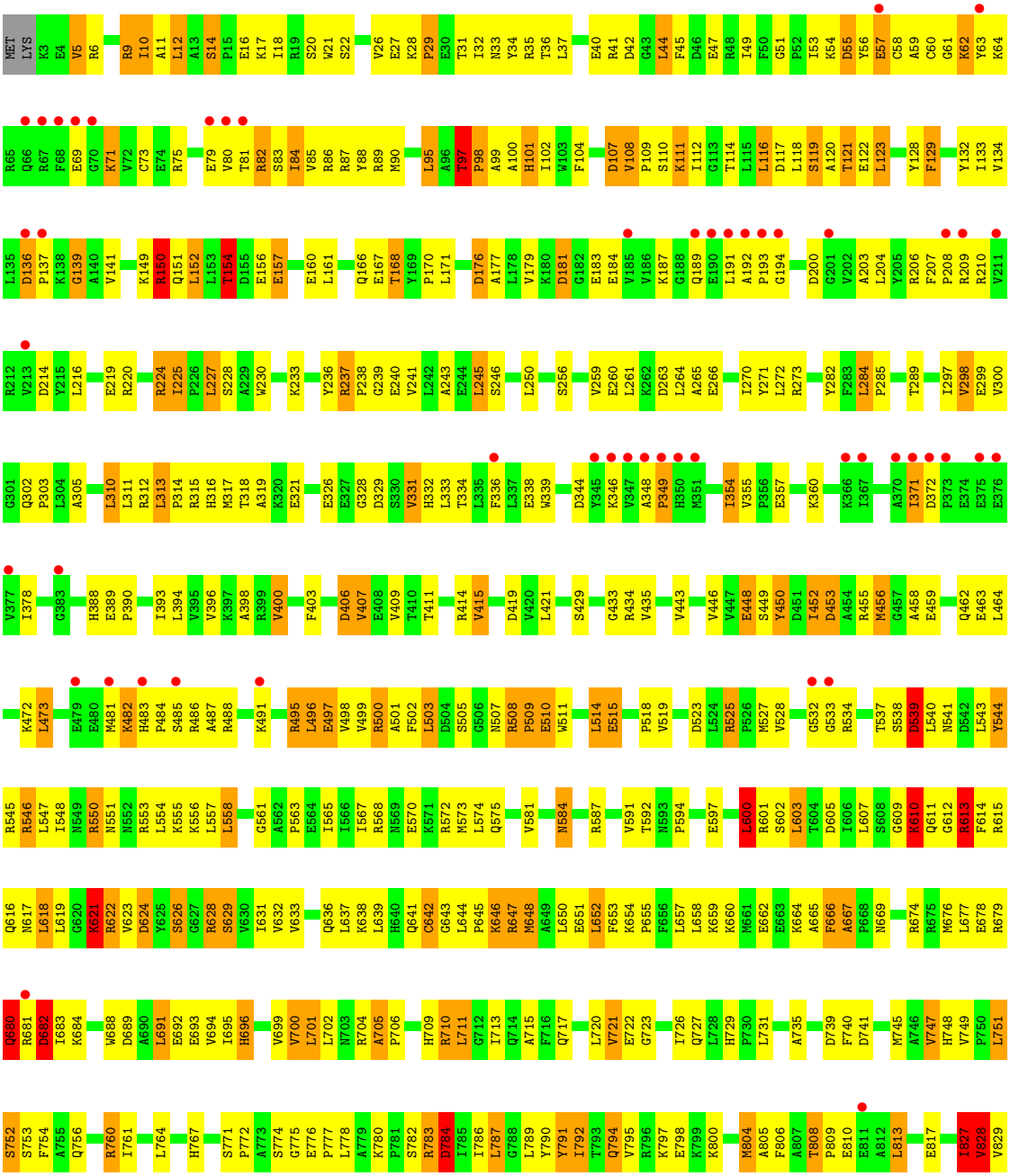


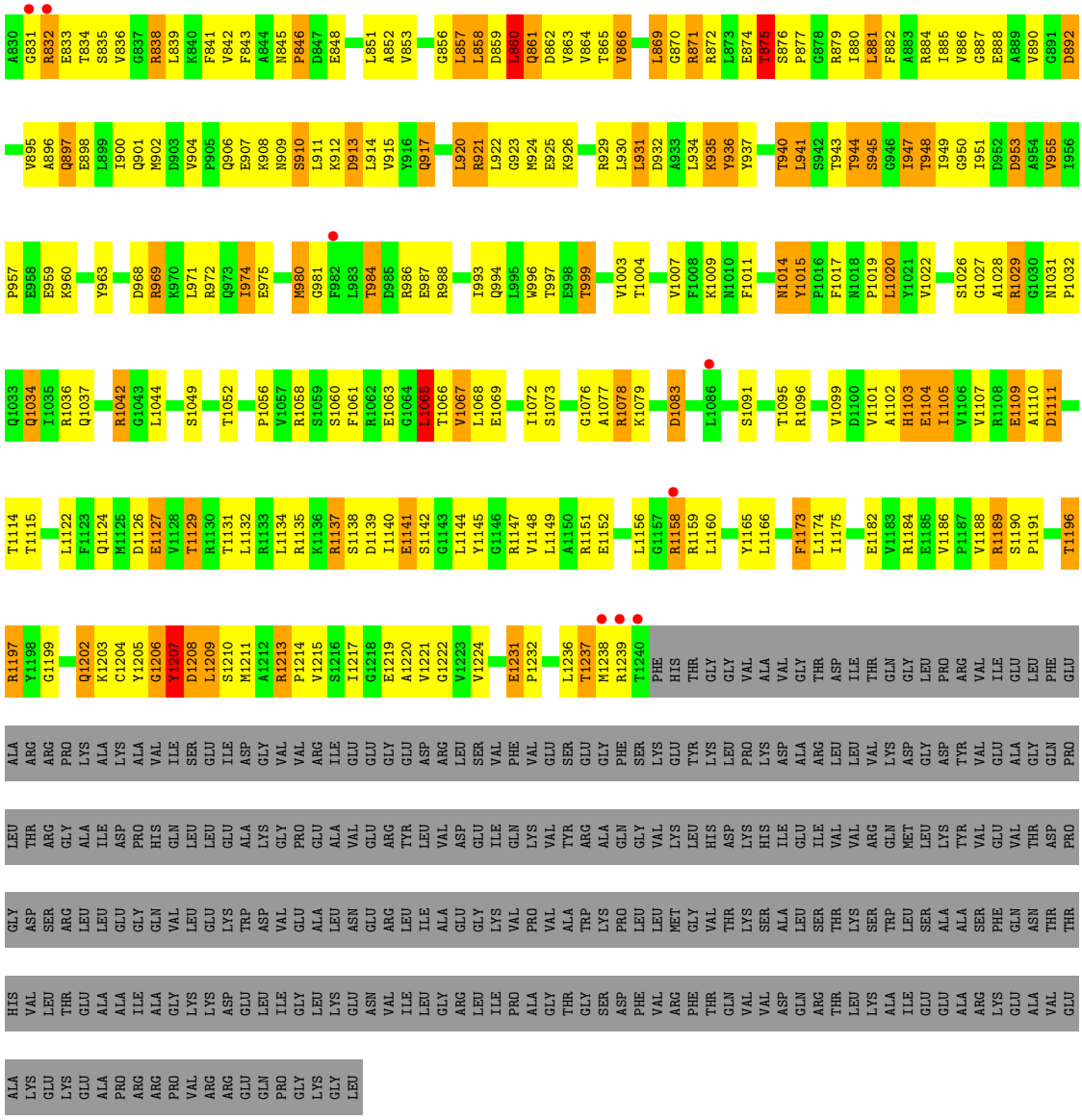


• Molecule 3: DNA-directed RNA polymerase beta' chain

Chain D:

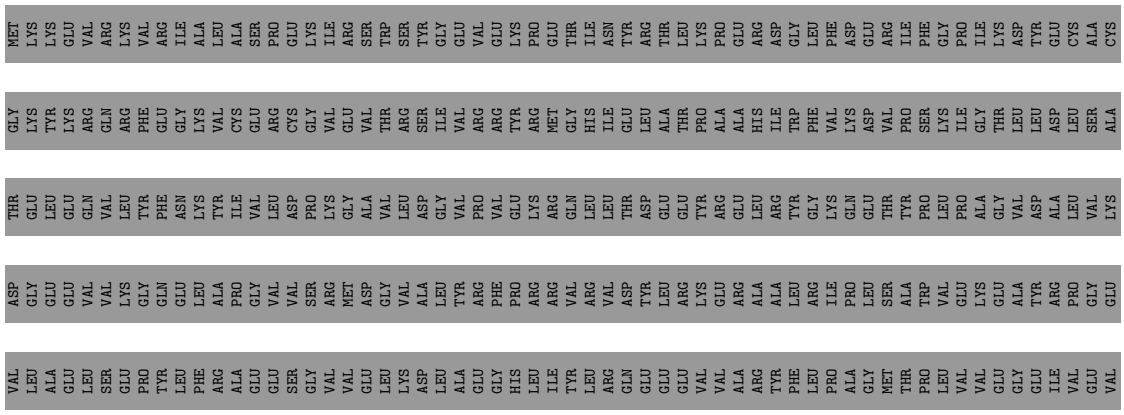


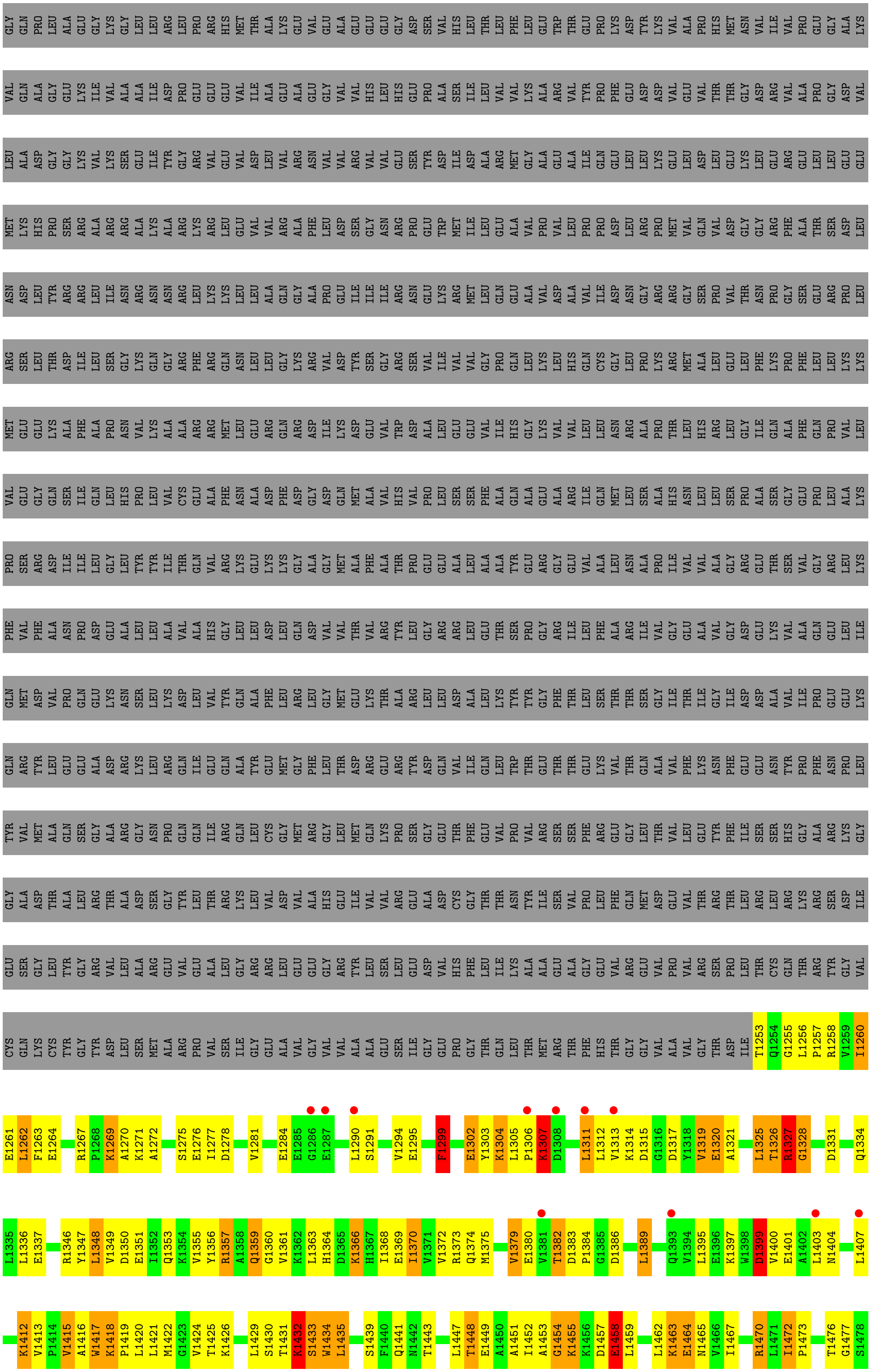


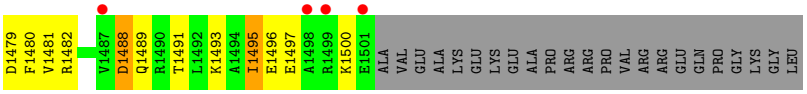


• Molecule 3: DNA-directed RNA polymerase beta' chain

Chain J:

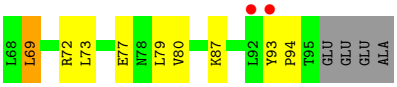






• Molecule 4: DNA-directed RNA polymerase omega chain

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	199.19Å 199.19Å 289.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 39.84 – 3.18	Depositor EDS
% Data completeness (in resolution range)	93.1 (40.00-3.20) 92.3 (39.84-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.281 , 0.346 0.259 , 0.260	Depositor DCC
R_{free} test set	4796 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	69.0	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 44.0	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	0.87	EDS
Total number of atoms	24369	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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: ZN, SRN

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	0.52	0/1798	0.88	10/2453 (0.4%)
1	B	0.52	0/1784	0.87	6/2428 (0.2%)
2	C	0.55	0/8744	0.88	35/11850 (0.3%)
3	D	0.52	0/9772	0.81	27/13234 (0.2%)
3	J	0.49	0/1897	0.81	7/2570 (0.3%)
4	K	0.52	0/762	0.79	1/1029 (0.1%)
All	All	0.53	0/24757	0.84	86/33564 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
3	D	0	2
All	All	0	5

There are no bond length outliers.

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	680	ASP	CB-CG-OD2	7.16	124.74	118.30
2	C	554	ASP	CB-CG-OD2	6.96	124.56	118.30
3	D	860	LEU	CA-CB-CG	6.92	131.22	115.30
2	C	492	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	193	ASP	CB-CG-OD2	6.71	124.34	118.30
1	B	18	ASP	CB-CG-OD2	6.67	124.31	118.30
2	C	133	ASP	CB-CG-OD2	6.67	124.30	118.30
2	C	863	ASP	CB-CG-OD2	6.63	124.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	868	ASP	CB-CG-OD2	6.55	124.20	118.30
1	A	113	ASP	CB-CG-OD2	6.54	124.18	118.30
3	D	263	ASP	CB-CG-OD2	6.51	124.16	118.30
2	C	968	ASP	CB-CG-OD2	6.43	124.09	118.30
2	C	1095	LEU	CA-CB-CG	6.42	130.07	115.30
3	J	1278	ASP	CB-CG-OD2	6.37	124.03	118.30
3	J	1317	ASP	CB-CG-OD2	6.34	124.01	118.30
2	C	300	ASP	CB-CG-OD2	6.34	124.00	118.30
3	D	892	ASP	CB-CG-OD2	6.18	123.87	118.30
3	D	600	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	60	ASP	CB-CG-OD2	6.07	123.76	118.30
2	C	429	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	145	ASP	CB-CG-OD2	5.95	123.66	118.30
3	D	739	ASP	CB-CG-OD2	5.94	123.65	118.30
3	J	1479	ASP	CB-CG-OD2	5.89	123.60	118.30
2	C	67	ASP	CB-CG-OD2	5.88	123.60	118.30
2	C	1103	ASP	CB-CG-OD2	5.86	123.57	118.30
3	J	1350	ASP	CB-CG-OD2	5.76	123.48	118.30
3	D	55	ASP	CB-CG-OD2	5.69	123.42	118.30
2	C	365	ASP	CB-CG-OD2	5.69	123.42	118.30
2	C	857	ASP	CB-CG-OD2	5.68	123.41	118.30
3	D	1065	LEU	CA-CB-CG	5.67	128.35	115.30
1	B	126	ASP	CB-CG-OD2	5.67	123.40	118.30
2	C	600	ASP	CB-CG-OD2	5.62	123.36	118.30
3	D	862	ASP	CB-CG-OD2	5.60	123.34	118.30
3	D	539	ASP	CB-CG-OD2	5.59	123.33	118.30
3	D	107	ASP	CB-CG-OD2	5.57	123.31	118.30
3	D	372	ASP	CB-CG-OD2	5.53	123.28	118.30
4	K	14	ASP	CB-CG-OD2	5.51	123.26	118.30
2	C	104	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	145	ASP	CB-CG-OD2	5.46	123.21	118.30
2	C	976	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	113	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	202	ASP	CB-CG-OD2	5.42	123.17	118.30
2	C	753	ASP	CB-CG-OD2	5.41	123.17	118.30
2	C	950	LEU	CA-CB-CG	5.38	127.67	115.30
3	D	953	ASP	CB-CG-OD2	5.38	123.14	118.30
3	J	1386	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	191	ASP	CB-CG-OD2	5.35	123.11	118.30
3	D	523	ASP	CB-CG-OD2	5.34	123.11	118.30
3	J	1399	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	197	LEU	CA-CB-CG	5.33	127.56	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	119	ASP	CB-CG-OD2	5.31	123.08	118.30
2	C	111	ASP	CB-CG-OD2	5.31	123.08	118.30
2	C	1059	ASP	CB-CG-OD2	5.28	123.05	118.30
2	C	223	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	160	ASP	CB-CG-OD2	5.27	123.04	118.30
2	C	324	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	18	ASP	CB-CG-OD2	5.22	123.00	118.30
2	C	246	ASP	CB-CG-OD2	5.21	122.99	118.30
3	D	406	ASP	CB-CG-OD2	5.21	122.99	118.30
3	D	1083	ASP	CB-CG-OD2	5.21	122.99	118.30
3	D	1126	ASP	CB-CG-OD2	5.21	122.99	118.30
3	D	682	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	60	ASP	CB-CG-OD2	5.19	122.97	118.30
2	C	969	LEU	CA-CB-CG	5.18	127.22	115.30
3	D	200	ASP	CB-CG-OD2	5.16	122.95	118.30
2	C	937	ASP	CB-CG-OD2	5.16	122.94	118.30
3	D	968	ASP	CB-CG-OD2	5.13	122.92	118.30
2	C	52	PHE	N-CA-C	5.13	124.85	111.00
1	A	193	ASP	CB-CG-OD2	5.13	122.91	118.30
3	D	1139	ASP	CB-CG-OD2	5.13	122.91	118.30
2	C	264	PRO	N-CD-CG	-5.12	95.52	103.20
2	C	30	LEU	CA-CB-CG	5.11	127.05	115.30
3	D	214	ASP	CB-CG-OD2	5.11	122.90	118.30
3	D	605	ASP	CB-CG-OD2	5.11	122.90	118.30
2	C	1106	ASP	CB-CG-OD2	5.10	122.89	118.30
2	C	657	ASP	CB-CG-OD2	5.09	122.89	118.30
3	D	453	ASP	CB-CG-OD2	5.09	122.89	118.30
3	D	181	ASP	CB-CG-OD2	5.08	122.88	118.30
2	C	216	ASP	CB-CG-OD2	5.08	122.87	118.30
3	D	31	THR	N-CA-C	5.05	124.65	111.00
2	C	151	ASP	CB-CG-OD2	5.05	122.85	118.30
2	C	295	ASP	CB-CG-OD2	5.05	122.84	118.30
3	D	329	ASP	CB-CG-OD2	5.05	122.84	118.30
3	J	1315	ASP	CB-CG-OD2	5.03	122.83	118.30
3	D	851	LEU	CA-CB-CG	5.02	126.84	115.30
2	C	590	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	1076	VAL	Peptide

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Mol	Chain	Res	Type	Group
2	C	213	ALA	Peptide
2	C	671	ASN	Peptide
3	D	1207	TYR	Peptide
3	D	21	TRP	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	1763	0	1760	117	0
1	B	1750	0	1775	77	0
2	C	8578	0	8517	538	0
3	D	9602	0	9556	504	0
3	J	1869	0	1876	88	0
4	K	747	0	735	41	0
5	C	58	0	64	5	0
6	D	2	0	0	0	0
All	All	24369	0	24283	1265	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 26.

All (1265) 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:705:ALA:CB	3:D:706:PRO:HD3	1.72	1.17
3:D:643:GLY:HA3	3:D:727:GLN:H	1.12	1.15
2:C:263:ASP:HB3	2:C:264:PRO:HD3	1.18	1.12
3:D:1110:ALA:HA	3:D:1202:GLN:HB3	1.33	1.09
3:D:551:ASN:O	3:D:555:LYS:HB2	1.51	1.08
3:D:699:VAL:H	3:D:756:GLN:NE2	1.52	1.07
2:C:710:ILE:HD11	2:C:758:ARG:HD3	1.35	1.06
2:C:881:ASN:H	2:C:881:ASN:ND2	1.49	1.04
2:C:881:ASN:HD22	2:C:881:ASN:N	1.50	1.03
3:D:705:ALA:HB1	3:D:706:PRO:HD3	1.37	1.03
3:D:1068:LEU:O	3:D:1072:ILE:HG12	1.58	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:98:PRO:HB2	3:D:458:ALA:HB3	1.41	1.03
1:A:201:THR:HG21	1:A:205:VAL:O	1.58	1.02
1:B:26:GLU:HB3	1:B:27:PRO:HD3	1.40	1.02
3:J:1276:GLU:HG3	3:J:1303:TYR:OH	1.59	1.01
3:D:1209:LEU:HG	3:D:1211:MET:SD	2.00	1.01
4:K:59:ASN:HD21	4:K:61:VAL:HG23	1.20	1.00
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	1.44	0.99
3:D:783:ARG:O	3:D:784:ASP:HB2	1.63	0.98
3:J:1432:LYS:HG2	3:J:1433:SER:H	1.27	0.96
3:J:1462:LEU:HB3	3:J:1472:ILE:HD11	1.45	0.96
3:D:705:ALA:CB	3:D:706:PRO:CD	2.45	0.95
3:D:828:VAL:HG11	3:D:863:VAL:H	1.32	0.94
1:A:206:THR:HB	1:A:209:GLU:HG3	1.48	0.94
3:D:136:ASP:HB3	3:D:137:PRO:HD3	1.47	0.93
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.50	0.93
3:D:699:VAL:H	3:D:756:GLN:HE21	1.11	0.93
1:B:26:GLU:CB	1:B:27:PRO:HD3	1.99	0.92
3:D:705:ALA:HB3	3:D:706:PRO:HD3	1.49	0.91
4:K:34:ARG:O	4:K:36:LYS:N	2.03	0.91
1:A:20:TYR:HD2	1:A:21:GLY:N	1.67	0.91
3:D:136:ASP:CB	3:D:137:PRO:HD3	2.01	0.91
3:D:774:SER:O	3:D:776:GLU:N	2.04	0.90
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.05	0.89
2:C:258:PHE:HD1	2:C:258:PHE:H	1.11	0.89
1:A:202:ASP:O	1:A:204:SER:N	2.06	0.89
3:D:804:MET:HG3	3:D:805:ALA:H	1.36	0.89
1:B:29:GLU:OE1	1:B:189:ARG:NH2	2.06	0.89
3:J:1326:THR:O	3:J:1327:ARG:HB2	1.71	0.88
1:A:138:LEU:HG	1:A:140:MET:HE1	1.54	0.88
2:C:1067:TYR:CE2	2:C:1071:ILE:HD11	2.09	0.88
3:D:97:THR:CB	3:D:98:PRO:HD3	2.05	0.87
2:C:358:ARG:HE	2:C:374:ASN:HD21	1.23	0.86
2:C:263:ASP:CB	2:C:264:PRO:HD3	2.03	0.86
3:D:805:ALA:HB3	3:D:832:ARG:H	1.40	0.86
3:D:509:PRO:O	3:D:510:GLU:HG3	1.74	0.86
1:A:55:SER:HB2	1:A:166:PRO:HA	1.58	0.86
1:A:233:LEU:HD12	1:A:234:PRO:HD2	1.57	0.86
3:D:525:ARG:NH1	3:D:541:ASN:OD1	2.08	0.85
3:D:210:ARG:HD2	3:D:344:ASP:HB3	1.59	0.85
3:D:137:PRO:HD2	3:D:453:ASP:HB3	1.59	0.85
3:D:984:THR:HG23	3:D:987:GLU:HB2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:397:GLU:H	2:C:633:GLN:NE2	1.74	0.84
2:C:1075:ASP:O	2:C:1076:VAL:HB	1.75	0.84
2:C:577:PRO:HA	2:C:671:ASN:ND2	1.93	0.84
2:C:281:LEU:HD11	2:C:306:THR:HA	1.60	0.84
2:C:263:ASP:HB3	2:C:264:PRO:CD	2.07	0.84
2:C:142:ARG:HG2	2:C:142:ARG:HH11	1.43	0.83
2:C:328:LEU:HB2	2:C:433:THR:HG21	1.60	0.83
2:C:577:PRO:HA	2:C:671:ASN:HD22	1.43	0.83
3:J:1263:PHE:O	3:J:1424:VAL:HB	1.79	0.83
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.62	0.81
2:C:258:PHE:N	2:C:258:PHE:CD1	2.49	0.81
3:D:610:LYS:O	3:D:610:LYS:HG2	1.80	0.81
2:C:640:ARG:HH11	2:C:642:ARG:HH22	1.28	0.80
2:C:859:PRO:CB	2:C:974:LEU:HD13	2.11	0.80
2:C:1056:LYS:HD3	3:D:751:LEU:HD21	1.61	0.80
1:B:26:GLU:HB3	1:B:27:PRO:CD	2.10	0.80
1:A:138:LEU:HG	1:A:140:MET:CE	2.10	0.80
2:C:1008:ARG:HH12	2:C:1012:PRO:HD2	1.46	0.80
1:B:44:LEU:O	1:B:174:VAL:HG21	1.82	0.80
3:D:409:VAL:HG12	3:D:435:VAL:HG11	1.63	0.80
3:D:705:ALA:HB3	3:D:706:PRO:CD	2.09	0.80
2:C:859:PRO:HB2	2:C:974:LEU:HD13	1.64	0.80
3:D:957:PRO:HD3	3:D:1007:VAL:HG23	1.64	0.80
3:D:1205:TYR:CE1	3:J:1366:LYS:HD3	2.17	0.80
1:A:30:ARG:HH22	3:D:856:GLY:H	1.31	0.79
2:C:397:GLU:HB2	2:C:633:GLN:HE21	1.47	0.79
2:C:393:GLN:HG3	2:C:406:HIS:HE1	1.47	0.79
3:D:509:PRO:C	3:D:510:GLU:HG3	2.01	0.79
2:C:327:HIS:HD2	2:C:329:GLY:H	1.28	0.79
2:C:1008:ARG:HD2	2:C:1028:GLY:O	1.83	0.79
2:C:227:LEU:HD21	2:C:237:ARG:HE	1.46	0.78
3:D:139:GLY:HA2	3:D:452:ILE:HG22	1.64	0.78
3:J:1457:ASP:O	3:J:1458:GLU:HB2	1.83	0.78
2:C:876:VAL:O	2:C:879:ARG:O	2.02	0.78
2:C:1034:GLU:HB3	3:D:618:LEU:O	1.83	0.78
1:B:44:LEU:HD13	1:B:214:ALA:HB2	1.65	0.78
3:D:36:THR:HG22	3:D:37:LEU:H	1.49	0.78
3:D:643:GLY:HA3	3:D:727:GLN:N	1.96	0.77
3:D:647:ARG:NH2	3:D:683:ILE:HD11	1.99	0.77
3:D:959:GLU:HB3	3:D:963:TYR:CD1	2.19	0.77
1:A:20:TYR:CD2	1:A:21:GLY:N	2.53	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:715:THR:HG21	3:D:533:GLY:H	1.50	0.77
2:C:768:SER:O	2:C:769:PRO:O	2.02	0.77
4:K:59:ASN:ND2	4:K:61:VAL:HG23	1.97	0.77
3:D:1207:TYR:HA	3:D:1213:ARG:O	1.84	0.77
3:D:58:CYS:SG	3:D:59:ALA:N	2.58	0.77
3:D:150:ARG:O	3:D:150:ARG:HG2	1.83	0.77
2:C:142:ARG:HH11	2:C:142:ARG:CG	1.97	0.77
3:D:804:MET:HG3	3:D:805:ALA:N	1.99	0.76
2:C:142:ARG:HG2	2:C:142:ARG:NH1	1.98	0.76
2:C:13:ILE:HD11	2:C:483:VAL:HG21	1.67	0.76
2:C:148:PHE:CZ	2:C:309:TYR:HB3	2.20	0.76
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.14	0.76
3:D:806:PHE:HB2	3:D:808:THR:O	1.85	0.76
4:K:59:ASN:HD21	4:K:61:VAL:CG2	1.98	0.76
2:C:809:GLY:O	2:C:810:ASP:O	2.04	0.76
3:D:561:GLY:O	3:D:563:PRO:HD3	1.86	0.76
2:C:1021:LEU:HG	3:D:622:ARG:HD2	1.66	0.76
2:C:717:LEU:HD21	3:D:35:ARG:HA	1.68	0.75
2:C:110:GLU:HB2	2:C:369:PRO:HG2	1.68	0.75
1:A:206:THR:HG22	1:A:208:LEU:H	1.52	0.75
2:C:393:GLN:HG3	2:C:406:HIS:CE1	2.21	0.75
2:C:872:ASN:OD1	2:C:874:LEU:HB2	1.86	0.75
3:D:767:HIS:HE1	4:K:3:GLU:H	1.34	0.75
1:B:150:TYR:HD1	1:B:170:ILE:HG23	1.52	0.75
2:C:471:TYR:OH	2:C:516:ARG:NH2	2.20	0.75
2:C:227:LEU:HD13	2:C:229:MET:HB2	1.69	0.74
3:D:1197:ARG:HH22	3:J:1374:GLN:NE2	1.85	0.74
3:D:813:LEU:HD11	3:D:839:LEU:HD13	1.67	0.74
2:C:376:ARG:H	2:C:377:PRO:HD3	1.52	0.74
2:C:285:LEU:HD21	2:C:302:VAL:HG23	1.70	0.74
2:C:548:PRO:HA	2:C:581:THR:CG2	2.18	0.74
2:C:399:ASN:ND2	2:C:402:SER:H	1.86	0.74
4:K:59:ASN:HD22	4:K:62:THR:H	1.34	0.74
4:K:59:ASN:ND2	4:K:62:THR:H	1.86	0.73
3:D:220:ARG:HH21	3:D:336:PHE:HB2	1.54	0.73
2:C:841:ASN:C	2:C:841:ASN:HD22	1.90	0.73
3:D:191:LEU:HD22	3:D:393:ILE:HG21	1.71	0.73
2:C:710:ILE:HB	2:C:790:LEU:HD13	1.69	0.73
2:C:710:ILE:HD11	2:C:758:ARG:CD	2.17	0.73
3:D:609:GLY:HA3	3:D:615:ARG:HH21	1.52	0.73
2:C:73:ILE:HG13	2:C:94:LEU:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1465:ASN:ND2	3:J:1470:ARG:HD3	2.04	0.73
2:C:889:HIS:HE1	3:D:951:ILE:H	1.37	0.73
3:D:805:ALA:HB1	3:D:834:THR:H	1.52	0.73
2:C:193:LEU:HD22	2:C:197:LEU:HG	1.69	0.72
2:C:266:ARG:O	2:C:268:ASP:N	2.22	0.72
2:C:96:ALA:CB	2:C:115:LEU:HD11	2.19	0.72
3:J:1413:VAL:HG12	3:J:1415:VAL:H	1.53	0.72
2:C:39:ARG:HB3	2:C:45:GLN:HG3	1.71	0.72
2:C:222:LEU:O	2:C:224:GLU:N	2.21	0.72
3:D:1211:MET:HG3	3:D:1213:ARG:HD2	1.71	0.72
2:C:149:THR:HG22	2:C:150:PRO:HD2	1.72	0.72
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.72	0.72
2:C:184:MET:HE3	2:C:191:PHE:HZ	1.54	0.72
3:D:852:ALA:O	3:D:857:LEU:HB2	1.90	0.72
1:A:201:THR:CG2	1:A:205:VAL:O	2.38	0.72
2:C:522:VAL:HG12	2:C:524:VAL:HG23	1.71	0.72
2:C:691:SER:OG	2:C:693:GLU:HB3	1.90	0.72
3:D:97:THR:HB	3:D:98:PRO:HD3	1.71	0.72
2:C:292:ARG:O	2:C:294:GLU:N	2.22	0.72
3:D:551:ASN:O	3:D:555:LYS:CB	2.34	0.72
3:J:1432:LYS:HG2	3:J:1433:SER:N	2.03	0.72
3:D:828:VAL:CG1	3:D:863:VAL:H	2.03	0.71
3:D:97:THR:HB	3:D:98:PRO:CD	2.20	0.71
3:D:908:LYS:HB2	3:D:1027:GLY:CA	2.20	0.71
1:A:157:GLY:O	1:A:158:ILE:HD13	1.89	0.71
3:D:1107:VAL:HG12	3:D:1217:ILE:HA	1.73	0.71
3:D:804:MET:CG	3:D:805:ALA:N	2.53	0.71
1:A:195:LEU:HD22	1:A:196:THR:N	2.06	0.71
3:D:225:ILE:HD12	3:D:230:TRP:HB2	1.71	0.71
3:D:892:ASP:OD1	3:D:895:VAL:N	2.17	0.71
1:A:57:TYR:HB3	1:A:141:GLU:HB2	1.72	0.70
1:A:83:LYS:HE3	1:A:168:ASP:HB2	1.73	0.70
1:A:233:LEU:HD13	1:B:14:THR:HG21	1.72	0.70
3:D:1037:GLN:HE21	3:D:1042:ARG:HE	1.39	0.70
2:C:80:GLN:HE22	2:C:122:THR:HG23	1.56	0.70
2:C:548:PRO:HA	2:C:581:THR:HG22	1.73	0.70
2:C:698:ASP:OD2	2:C:701:THR:HG21	1.91	0.70
2:C:1052:MET:HG3	3:D:623:VAL:HG21	1.71	0.70
2:C:762:LYS:HD2	2:C:786:LYS:HD3	1.72	0.70
3:J:1465:ASN:HD22	3:J:1470:ARG:HD3	1.56	0.70
2:C:1088:LEU:HA	3:D:613:ARG:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:ARG:C	2:C:268:ASP:H	1.94	0.70
1:B:150:TYR:CD1	1:B:170:ILE:HG23	2.27	0.70
2:C:257:LEU:O	2:C:264:PRO:HG2	1.91	0.70
2:C:715:THR:CG2	3:D:533:GLY:H	2.05	0.70
3:D:71:LYS:HG3	3:D:80:VAL:HB	1.74	0.70
2:C:640:ARG:NH1	2:C:642:ARG:HH22	1.90	0.70
3:D:1231:GLU:HG3	3:D:1232:PRO:HD3	1.74	0.70
1:A:26:GLU:OE1	1:A:194:LYS:HG3	1.92	0.70
3:D:871:ARG:HG3	3:D:871:ARG:HH11	1.56	0.70
2:C:154:ARG:HH22	2:C:157:ARG:NH1	1.89	0.69
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.71	0.69
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.22	0.69
1:B:179:PHE:CD1	1:B:179:PHE:C	2.64	0.69
3:D:699:VAL:N	3:D:756:GLN:NE2	2.34	0.69
3:D:805:ALA:HB3	3:D:832:ARG:N	2.07	0.69
1:A:21:GLY:O	1:A:198:ARG:O	2.10	0.69
2:C:261:LEU:HG	2:C:263:ASP:H	1.57	0.69
2:C:769:PRO:O	2:C:771:GLU:N	2.24	0.69
1:A:190:THR:CG2	1:A:190:THR:O	2.40	0.69
3:D:550:ARG:HD2	3:D:573:MET:HB3	1.74	0.69
3:D:227:LEU:HD22	3:D:331:VAL:HG22	1.74	0.69
3:D:721:VAL:HG21	3:D:727:GLN:NE2	2.08	0.69
3:D:790:TYR:CE2	3:D:794:GLN:HG3	2.27	0.69
2:C:159:ILE:HG22	2:C:175:GLU:HB3	1.73	0.69
2:C:397:GLU:H	2:C:633:GLN:HE21	1.39	0.69
2:C:700:TYR:CB	2:C:833:LEU:HD22	2.23	0.69
2:C:743:VAL:HG22	2:C:755:LEU:O	1.92	0.69
2:C:184:MET:HE1	2:C:196:LEU:HD22	1.72	0.69
3:D:731:LEU:HD11	3:D:935:LYS:HB2	1.74	0.69
2:C:910:THR:H	2:C:913:GLU:HG3	1.59	0.68
3:D:971:LEU:O	3:D:974:ILE:HG22	1.92	0.68
3:J:1462:LEU:HB3	3:J:1472:ILE:CD1	2.23	0.68
3:J:1472:ILE:HG13	3:J:1473:PRO:HD2	1.75	0.68
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.92	0.68
3:D:806:PHE:CD1	3:D:809:PRO:HA	2.27	0.68
2:C:1018:GLN:HG2	2:C:1060:ILE:HD11	1.75	0.68
3:D:937:TYR:O	3:D:941:LEU:HB2	1.93	0.68
1:A:86:VAL:HG22	1:A:123:MET:HB2	1.75	0.68
1:B:44:LEU:HB3	1:B:177:VAL:HG21	1.75	0.68
2:C:904:PRO:HB2	2:C:907:ASP:HB3	1.76	0.68
3:D:136:ASP:CG	3:D:137:PRO:HD3	2.13	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:171:LEU:HD12	3:D:390:PRO:O	1.93	0.68
2:C:981:GLU:HG3	2:C:982:PRO:HD2	1.76	0.67
2:C:487:THR:HG22	2:C:489:SER:H	1.60	0.67
2:C:1012:PRO:HG2	2:C:1023:GLY:HA2	1.76	0.67
3:D:1031:ASN:OD1	3:D:1034:GLN:NE2	2.28	0.67
1:A:233:LEU:HD13	1:B:14:THR:CG2	2.25	0.67
2:C:788:THR:O	2:C:788:THR:OG1	2.13	0.67
1:B:175:ARG:HH11	1:B:202:ASP:HA	1.59	0.67
2:C:878:SER:HB2	3:D:1029:ARG:HD3	1.77	0.67
3:D:136:ASP:HB3	3:D:137:PRO:CD	2.21	0.66
1:B:43:ILE:HD13	1:B:218:LEU:HB2	1.78	0.66
3:D:871:ARG:HG3	3:D:871:ARG:NH1	2.08	0.66
2:C:148:PHE:HA	2:C:160:ALA:HA	1.76	0.66
2:C:397:GLU:N	2:C:633:GLN:HE21	1.94	0.66
3:D:36:THR:HG22	3:D:37:LEU:N	2.11	0.66
2:C:376:ARG:H	2:C:377:PRO:CD	2.08	0.66
2:C:872:ASN:OD1	2:C:874:LEU:N	2.28	0.66
3:D:871:ARG:HH11	3:D:871:ARG:CG	2.08	0.66
2:C:831:ARG:O	2:C:832:LYS:HB2	1.95	0.66
3:D:783:ARG:HG3	3:D:783:ARG:HH11	1.59	0.66
3:D:129:PHE:HA	3:D:572:ARG:HG3	1.77	0.66
1:B:24:VAL:HG22	1:B:196:THR:HG23	1.76	0.65
2:C:397:GLU:N	2:C:633:GLN:NE2	2.43	0.65
3:D:806:PHE:CG	3:D:809:PRO:HA	2.31	0.65
2:C:553:ASP:OD2	2:C:843:HIS:ND1	2.26	0.65
3:D:95:LEU:HB2	3:D:515:GLU:O	1.96	0.65
2:C:710:ILE:CD1	2:C:758:ARG:HD3	2.21	0.65
3:D:26:VAL:C	3:D:28:LYS:H	1.99	0.65
1:B:20:TYR:HA	1:B:199:ILE:O	1.97	0.65
2:C:257:LEU:HD23	2:C:264:PRO:HG3	1.79	0.65
3:D:643:GLY:CA	3:D:727:GLN:H	1.99	0.65
2:C:96:ALA:HB2	2:C:115:LEU:HD11	1.78	0.65
2:C:543:ASN:HA	2:C:546:LEU:HD12	1.78	0.65
2:C:127:PHE:CE1	2:C:386:PHE:HE2	2.15	0.65
2:C:261:LEU:HD21	2:C:263:ASP:HB3	1.78	0.65
3:D:318:THR:HG22	3:D:338:GLU:HB2	1.79	0.65
3:D:1207:TYR:O	3:D:1209:LEU:N	2.30	0.64
2:C:601:GLY:HA3	2:C:615:TYR:HA	1.79	0.64
2:C:918:LEU:HD22	2:C:967:PHE:O	1.96	0.64
3:D:1135:ARG:HB2	3:D:1140:ILE:HD11	1.78	0.64
2:C:1030:GLN:HB2	3:D:626:SER:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:246:ASP:OD1	2:C:246:ASP:N	2.31	0.64
2:C:560:MET:O	2:C:564:MET:HB2	1.98	0.64
2:C:775:ARG:HD2	2:C:782:ALA:HB2	1.78	0.64
3:J:1349:VAL:HG22	3:J:1368:ILE:HG22	1.78	0.64
3:D:433:GLY:HA2	3:D:449:SER:O	1.97	0.64
1:B:83:LYS:HB3	1:B:170:ILE:HD11	1.78	0.64
2:C:979:THR:O	2:C:981:GLU:N	2.31	0.64
2:C:1067:TYR:CZ	2:C:1071:ILE:HD11	2.32	0.64
3:D:136:ASP:CB	3:D:137:PRO:CD	2.74	0.64
3:D:959:GLU:HB3	3:D:963:TYR:HD1	1.63	0.64
2:C:809:GLY:O	2:C:810:ASP:C	2.36	0.64
1:A:20:TYR:HE2	1:A:22:GLU:HG3	1.61	0.64
3:J:1306:PRO:O	3:J:1307:LYS:HB3	1.97	0.64
3:J:1256:LEU:O	3:J:1260:ILE:HG12	1.98	0.63
3:J:1372:VAL:HA	3:J:1375:MET:HG3	1.81	0.63
2:C:95:TYR:HA	2:C:113:VAL:O	1.98	0.63
1:B:54:THR:CG2	1:B:143:ARG:HG2	2.28	0.63
3:D:168:THR:O	3:D:170:PRO:HD3	1.98	0.63
3:D:843:PHE:HB2	3:D:866:VAL:HG22	1.80	0.63
2:C:679:PHE:O	3:D:943:THR:OG1	2.16	0.63
3:J:1379:VAL:HG12	3:J:1418:LYS:O	1.99	0.63
2:C:141:HIS:CE1	2:C:332:ARG:HH11	2.17	0.63
3:D:699:VAL:N	3:D:756:GLN:HE21	1.91	0.63
3:D:761:ILE:O	3:D:767:HIS:HD2	1.82	0.63
3:D:999:THR:O	3:D:1003:VAL:HG23	1.99	0.63
2:C:650:LYS:HB2	2:C:653:ASP:HB2	1.81	0.62
1:A:181:VAL:O	2:C:937:ASP:HB2	1.99	0.62
2:C:327:HIS:CD2	2:C:329:GLY:H	2.15	0.62
3:D:538:SER:O	3:D:539:ASP:CB	2.47	0.62
3:D:558:LEU:HD22	3:D:567:ILE:HG12	1.82	0.62
3:D:26:VAL:HG12	3:D:26:VAL:O	1.98	0.62
2:C:31:GLN:H	2:C:31:GLN:HE21	1.46	0.62
2:C:815:LEU:HD13	2:C:819:VAL:HG12	1.81	0.62
1:A:111:ALA:HB2	1:A:127:LEU:HD23	1.80	0.62
2:C:164:PRO:HB3	2:C:265:LYS:CD	2.29	0.62
2:C:682:TYR:CE1	2:C:851:LYS:HE2	2.34	0.62
2:C:890:LEU:HD11	2:C:901:TYR:CE2	2.33	0.62
3:D:617:ASN:OD1	3:D:621:LYS:HE3	2.00	0.62
2:C:944:LEU:HD21	2:C:963:LEU:HD23	1.82	0.62
3:J:1353:GLN:O	3:J:1357:ARG:HB2	2.00	0.62
1:B:126:ASP:O	1:B:127:LEU:CB	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:95:TYR:HB3	2:C:112:GLU:HB3	1.82	0.62
1:A:89:PHE:O	1:A:119:ASP:O	2.18	0.61
2:C:790:LEU:O	2:C:791:ARG:HB2	2.00	0.61
3:D:225:ILE:O	3:D:331:VAL:HG23	2.00	0.61
3:D:45:PHE:O	3:D:86:ARG:NH2	2.33	0.61
3:D:1060:SER:O	3:D:1063:GLU:HG2	1.99	0.61
3:D:1122:LEU:HD11	3:D:1186:VAL:HG23	1.82	0.61
2:C:859:PRO:HB2	2:C:974:LEU:CD1	2.30	0.61
3:D:495:ARG:O	3:D:499:VAL:HG23	2.00	0.61
3:D:700:VAL:HG12	3:D:748:HIS:O	2.00	0.61
3:D:691:LEU:O	3:D:694:VAL:HB	1.99	0.61
3:D:749:VAL:O	3:D:751:LEU:HD13	2.01	0.61
3:D:1158:ARG:HH11	3:D:1160:LEU:HD21	1.66	0.61
2:C:29:ALA:HA	2:C:43:GLY:HA3	1.82	0.61
3:D:317:MET:HG2	3:D:339:TRP:HB3	1.83	0.61
3:J:1480:PHE:O	4:K:18:ARG:NH2	2.33	0.61
3:D:612:GLY:O	3:D:614:PHE:N	2.29	0.61
2:C:540:PHE:CE1	2:C:906:PHE:HE1	2.18	0.61
2:C:804:LEU:HB3	2:C:824:ARG:HB2	1.82	0.60
3:D:875:THR:HG21	3:D:880:ILE:HG12	1.83	0.60
2:C:42:VAL:HG12	2:C:43:GLY:H	1.66	0.60
2:C:432:ARG:O	2:C:433:THR:CB	2.49	0.60
2:C:889:HIS:CE1	3:D:951:ILE:H	2.17	0.60
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.82	0.60
3:D:907:GLU:H	3:D:910:SER:HB3	1.67	0.60
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	1.81	0.60
3:D:208:PRO:HA	3:D:390:PRO:HA	1.81	0.60
3:D:613:ARG:HH22	3:D:616:GLN:NE2	1.99	0.60
1:A:190:THR:O	1:A:190:THR:HG22	2.01	0.60
1:A:222:LEU:HD12	1:B:215:VAL:HG13	1.82	0.60
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.83	0.60
2:C:39:ARG:HB3	2:C:45:GLN:CG	2.31	0.60
2:C:674:VAL:HG12	2:C:990:GLY:O	2.02	0.60
2:C:495:THR:H	2:C:530:GLU:HG3	1.64	0.60
2:C:1107:ASN:HB2	2:C:1108:PRO:CD	2.32	0.60
3:D:777:PRO:HG2	3:D:912:LYS:HG3	1.84	0.60
1:B:25:LEU:HD12	1:B:28:LEU:HD21	1.84	0.60
2:C:369:PRO:O	2:C:370:ALA:CB	2.50	0.60
4:K:31:LEU:HD13	4:K:60:ALA:HB2	1.84	0.60
1:A:102:ARG:HG3	1:A:139:TYR:HD1	1.67	0.60
4:K:26:ARG:HH11	4:K:29:GLN:HE21	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1462:LEU:HD23	3:J:1473:PRO:HG2	1.84	0.60
2:C:859:PRO:HB3	2:C:974:LEU:HD13	1.84	0.59
3:D:1231:GLU:N	3:D:1232:PRO:CD	2.65	0.59
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.84	0.59
3:D:947:ILE:HD13	3:D:947:ILE:H	1.67	0.59
1:A:44:LEU:HA	1:A:48:ILE:CD1	2.32	0.59
1:A:110:ARG:O	1:A:112:GLY:N	2.35	0.59
2:C:860:HIS:CE1	2:C:975:TYR:HB3	2.37	0.59
2:C:890:LEU:HD11	2:C:901:TYR:CD2	2.38	0.59
2:C:715:THR:C	2:C:717:LEU:H	2.06	0.59
1:A:71:VAL:HG22	1:A:132:LEU:HD22	1.84	0.59
1:B:26:GLU:CB	1:B:27:PRO:CD	2.73	0.59
1:B:118:ALA:O	1:B:119:ASP:OD1	2.21	0.59
2:C:140:ILE:HG22	2:C:333:ILE:HG12	1.84	0.59
2:C:149:THR:HG22	2:C:150:PRO:CD	2.32	0.59
3:D:224:ARG:HH11	3:D:332:HIS:HB2	1.66	0.59
1:A:36:LEU:HD13	1:B:225:PHE:HE1	1.66	0.59
2:C:96:ALA:HB3	2:C:115:LEU:HD11	1.83	0.59
2:C:369:PRO:O	2:C:370:ALA:HB3	2.02	0.59
2:C:684:PHE:HB3	3:D:633:VAL:HG21	1.84	0.59
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.38	0.59
3:D:1103:HIS:HD2	3:J:1462:LEU:H	1.51	0.59
2:C:127:PHE:CZ	2:C:386:PHE:HE2	2.21	0.58
1:B:44:LEU:HD13	1:B:214:ALA:CB	2.34	0.58
2:C:685:GLU:HB2	3:D:740:PHE:HD1	1.67	0.58
2:C:987:ILE:HA	3:D:948:THR:HG21	1.85	0.58
3:D:969:ARG:HH21	3:D:972:ARG:HD3	1.68	0.58
2:C:1077:PRO:HG3	3:D:752:SER:HB3	1.85	0.58
3:D:97:THR:OG1	3:D:98:PRO:HD3	2.03	0.58
3:D:539:ASP:OD1	3:D:600:LEU:HB2	2.03	0.58
1:B:183:ASP:N	1:B:183:ASP:OD1	2.35	0.58
2:C:254:LEU:HG	2:C:258:PHE:HE1	1.68	0.58
2:C:541:SER:O	2:C:545:ASN:HB2	2.02	0.58
2:C:876:VAL:HB	3:D:949:ILE:HD13	1.84	0.58
3:D:875:THR:HG23	3:D:876:SER:N	2.17	0.58
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.38	0.58
3:D:26:VAL:HG11	3:D:44:LEU:HD23	1.84	0.58
3:D:270:ILE:HB	3:D:282:TYR:HB2	1.86	0.58
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.86	0.58
1:B:25:LEU:CD1	1:B:28:LEU:HD21	2.33	0.58
2:C:343:GLN:HA	2:C:346:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:911:GLU:N	2:C:912:PRO:HD2	2.18	0.58
2:C:376:ARG:N	2:C:377:PRO:CD	2.66	0.58
2:C:399:ASN:HD21	2:C:402:SER:H	1.52	0.58
3:D:354:ILE:O	3:D:354:ILE:HG23	2.04	0.58
4:K:16:LYS:HG2	4:K:17:TYR:N	2.18	0.58
3:D:33:ASN:HD22	3:D:36:THR:HB	1.68	0.58
3:D:1066:THR:O	3:D:1068:LEU:N	2.36	0.58
2:C:86:LYS:O	2:C:87:ASP:HB2	2.04	0.57
2:C:749:VAL:HG12	2:C:792:VAL:HG21	1.85	0.57
3:D:1107:VAL:CG1	3:D:1217:ILE:HA	2.34	0.57
2:C:874:LEU:HD11	3:D:787:LEU:HD23	1.84	0.57
3:D:33:ASN:ND2	3:D:36:THR:HB	2.19	0.57
3:D:116:LEU:HB2	3:D:118:LEU:CD2	2.34	0.57
3:D:647:ARG:HH21	3:D:683:ILE:HD11	1.67	0.57
1:A:73:GLU:HG3	1:A:130:ALA:HA	1.85	0.57
2:C:139:GLN:HB3	2:C:391:LEU:HD21	1.86	0.57
2:C:810:ASP:HB3	2:C:813:VAL:CG2	2.34	0.57
3:D:527:MET:SD	3:D:537:THR:HG22	2.44	0.57
2:C:134:ARG:NH1	2:C:392:SER:O	2.38	0.57
2:C:1107:ASN:HB2	2:C:1108:PRO:HD2	1.86	0.57
3:D:791:TYR:HD2	3:D:945:SER:HG	1.52	0.57
3:D:1148:VAL:HG21	3:D:1203:LYS:O	2.04	0.57
3:D:859:ASP:O	3:D:861:GLN:N	2.33	0.57
1:A:225:PHE:CZ	1:B:25:LEU:CD2	2.87	0.57
2:C:18:LEU:HD22	2:C:542:LEU:HD21	1.86	0.57
2:C:198:ARG:NH2	2:C:229:MET:O	2.37	0.57
3:D:881:LEU:C	3:D:881:LEU:HD12	2.25	0.57
2:C:198:ARG:NH1	2:C:202:TYR:O	2.38	0.57
2:C:679:PHE:CE2	2:C:853:LEU:HD21	2.40	0.57
3:D:62:LYS:HG3	3:D:63:TYR:H	1.70	0.57
3:D:149:LYS:O	3:D:151:GLN:N	2.37	0.57
3:D:1109:GLU:OE1	3:D:1196:THR:HG21	2.05	0.57
3:D:1208:ASP:C	3:D:1210:SER:H	2.06	0.57
1:A:225:PHE:CZ	1:B:25:LEU:HD21	2.39	0.56
3:D:108:VAL:H	3:D:109:PRO:CD	2.17	0.56
3:D:123:LEU:HD11	3:D:152:LEU:HD13	1.88	0.56
3:D:133:ILE:HA	3:D:456:MET:HG3	1.87	0.56
3:D:705:ALA:HB1	3:D:706:PRO:CD	2.19	0.56
2:C:399:ASN:C	2:C:399:ASN:HD22	2.08	0.56
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.20	0.56
3:J:1276:GLU:HG3	3:J:1303:TYR:HH	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:575:GLN:HE21	2:C:671:ASN:H	1.52	0.56
3:D:1103:HIS:CD2	3:J:1463:LYS:H	2.22	0.56
1:A:108:GLU:O	1:A:110:ARG:HD3	2.05	0.56
2:C:492:ASP:HB3	2:C:518:ARG:HG2	1.86	0.56
2:C:758:ARG:O	2:C:787:ASP:O	2.24	0.56
3:D:701:LEU:O	3:D:747:VAL:HA	2.05	0.56
3:D:921:ARG:HG2	3:D:921:ARG:HH11	1.70	0.56
1:A:83:LYS:CE	1:A:168:ASP:HB2	2.36	0.56
2:C:700:TYR:HB2	2:C:833:LEU:HD22	1.87	0.56
1:A:63:HIS:O	1:A:66:SER:OG	2.24	0.56
1:B:126:ASP:O	1:B:127:LEU:HB3	2.06	0.56
2:C:3:ILE:HG21	2:C:902:ILE:HD12	1.87	0.56
2:C:396:ASP:OD2	5:C:1120:SRN:H22	2.06	0.56
1:B:185:ARG:HA	1:B:189:ARG:O	2.06	0.56
2:C:874:LEU:O	3:D:1029:ARG:HD2	2.06	0.56
3:D:482:LYS:C	3:D:484:PRO:HD3	2.26	0.56
3:D:1066:THR:O	3:D:1069:GLU:N	2.39	0.56
2:C:1023:GLY:HA3	2:C:1027:PHE:HA	1.87	0.55
3:D:57:GLU:N	3:D:80:VAL:HG13	2.21	0.55
3:D:508:ARG:C	3:D:509:PRO:O	2.43	0.55
3:D:689:ASP:O	3:D:693:GLU:HG3	2.06	0.55
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.87	0.55
3:J:1313:VAL:HG21	3:J:1325:LEU:HD12	1.89	0.55
4:K:8:LYS:HB3	4:K:69:LEU:HD11	1.89	0.55
1:A:133:GLU:HG2	1:A:134:GLU:N	2.20	0.55
1:B:175:ARG:NH1	1:B:202:ASP:HA	2.21	0.55
2:C:1058:ASP:O	2:C:1060:ILE:N	2.38	0.55
4:K:13:VAL:HG21	4:K:19:LEU:HB2	1.88	0.55
1:A:41:ARG:HG3	1:A:177:VAL:HG12	1.89	0.55
2:C:332:ARG:HH22	2:C:338:GLU:CD	2.09	0.55
3:D:1197:ARG:HH22	3:J:1374:GLN:HE22	1.54	0.55
2:C:697:ARG:HD2	2:C:699:PHE:CE1	2.42	0.55
3:D:805:ALA:CB	3:D:832:ARG:H	2.16	0.55
3:J:1260:ILE:O	3:J:1261:GLU:C	2.45	0.55
1:A:70:GLY:HA2	1:A:133:GLU:OE2	2.07	0.55
3:D:100:ALA:N	3:D:575:GLN:HE22	2.05	0.55
3:D:270:ILE:HD12	3:D:284:LEU:HD21	1.88	0.55
1:A:64:GLU:O	1:A:75:VAL:HB	2.07	0.55
3:D:507:ASN:ND2	3:J:1451:ALA:O	2.36	0.55
2:C:140:ILE:HG23	2:C:410:ILE:HG23	1.89	0.55
2:C:688:ILE:HG23	2:C:871:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ILE:CD1	1:B:218:LEU:HB2	2.36	0.55
2:C:715:THR:O	2:C:717:LEU:N	2.40	0.55
2:C:1056:LYS:HD3	3:D:751:LEU:CD2	2.33	0.55
3:D:1111:ASP:OD1	3:D:1189:ARG:NH1	2.39	0.55
3:D:859:ASP:C	3:D:861:GLN:H	2.10	0.55
2:C:628:TYR:H	2:C:638:ASP:HB2	1.73	0.54
3:D:10:ILE:HG13	3:D:11:ALA:N	2.22	0.54
1:A:20:TYR:HD2	1:A:20:TYR:C	2.11	0.54
3:D:666:PHE:O	3:D:667:ALA:CB	2.54	0.54
3:D:702:LEU:HB3	3:D:745:MET:CE	2.37	0.54
4:K:14:ASP:OD1	4:K:18:ARG:HD2	2.06	0.54
4:K:38:THR:HG23	4:K:40:LEU:CD2	2.37	0.54
1:B:170:ILE:HD13	3:D:848:GLU:HG3	1.89	0.54
2:C:852:ILE:HG13	2:C:852:ILE:O	2.07	0.54
3:D:543:LEU:HD21	3:D:600:LEU:HD11	1.88	0.54
3:D:1103:HIS:CD2	3:J:1462:LEU:H	2.25	0.54
2:C:432:ARG:O	2:C:433:THR:HB	2.08	0.54
2:C:487:THR:HG22	2:C:488:ALA:N	2.23	0.54
2:C:524:VAL:HG11	2:C:529:VAL:HG23	1.90	0.54
2:C:762:LYS:HE2	3:D:532:GLY:H	1.72	0.54
1:A:50:GLY:HA3	1:A:173:PRO:HD3	1.89	0.54
2:C:261:LEU:HD21	2:C:263:ASP:CB	2.37	0.54
3:D:835:SER:OG	3:D:838:ARG:HG2	2.07	0.54
3:D:1004:THR:O	3:D:1007:VAL:HG12	2.07	0.54
1:A:94:MET:SD	1:A:97:THR:HG22	2.48	0.54
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.89	0.54
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.89	0.54
2:C:474:VAL:HG12	2:C:479:VAL:HA	1.90	0.54
2:C:676:ILE:HA	2:C:871:LEU:O	2.08	0.54
3:J:1299:PHE:N	3:J:1299:PHE:CD2	2.76	0.54
1:A:211:LEU:O	1:A:215:VAL:HG12	2.07	0.54
3:J:1457:ASP:O	3:J:1458:GLU:CB	2.55	0.54
1:A:64:GLU:HG3	1:A:79:ILE:HD12	1.90	0.53
2:C:1051:GLU:HB3	2:C:1056:LYS:HE2	1.90	0.53
2:C:1088:LEU:HD12	3:D:613:ARG:HG3	1.89	0.53
5:C:1120:SRN:O1	5:C:1120:SRN:H4	2.08	0.53
3:D:936:TYR:CE2	3:D:940:THR:HG21	2.43	0.53
3:D:1031:ASN:HB2	3:D:1032:PRO:HD2	1.90	0.53
2:C:600:ASP:HB3	2:C:651:LYS:HA	1.90	0.53
2:C:712:ALA:HB1	2:C:720:GLU:O	2.09	0.53
2:C:749:VAL:CG1	2:C:792:VAL:HG21	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:203:ALA:O	3:D:204:LEU:HD23	2.09	0.53
3:D:137:PRO:HD2	3:D:453:ASP:CB	2.33	0.53
3:D:509:PRO:O	3:D:510:GLU:CG	2.51	0.53
2:C:22:GLN:NE2	2:C:136:ILE:O	2.41	0.53
2:C:1109:VAL:HG11	3:D:5:VAL:HG13	1.90	0.53
3:D:845:ASN:HB2	3:D:848:GLU:H	1.73	0.53
1:B:77:GLU:O	1:B:81:ASN:HB2	2.07	0.53
2:C:277:ALA:O	2:C:281:LEU:HB2	2.08	0.53
3:D:1231:GLU:HG3	3:D:1232:PRO:CD	2.38	0.53
3:J:1464:GLU:O	3:J:1467:ILE:HB	2.07	0.53
2:C:839:LEU:N	2:C:839:LEU:HD23	2.23	0.53
2:C:897:LEU:HD23	2:C:899:GLN:NE2	2.22	0.53
3:D:853:VAL:HG22	3:D:858:LEU:HD13	1.91	0.53
2:C:554:ASP:HB2	2:C:880:MET:HB2	1.91	0.53
2:C:897:LEU:HD23	2:C:899:GLN:CD	2.29	0.53
2:C:1067:TYR:CE2	2:C:1071:ILE:CD1	2.90	0.53
2:C:1075:ASP:O	2:C:1076:VAL:CB	2.52	0.53
4:K:15:SER:O	4:K:17:TYR:N	2.39	0.53
2:C:393:GLN:NE2	5:C:1120:SRN:C29	2.72	0.53
3:D:858:LEU:CD2	3:D:864:VAL:HG21	2.38	0.53
3:D:921:ARG:HH11	3:D:921:ARG:CG	2.22	0.53
2:C:1040:LEU:HD12	2:C:1049:LEU:HA	1.90	0.53
3:D:1135:ARG:HB2	3:D:1140:ILE:CD1	2.38	0.53
2:C:16:PRO:O	2:C:18:LEU:N	2.42	0.53
2:C:886:LEU:HG	3:D:951:ILE:HD12	1.90	0.53
3:D:101:HIS:HB3	3:D:104:PHE:HD1	1.72	0.53
3:D:157:GLU:O	3:D:161:LEU:HB2	2.10	0.52
3:D:166:GLN:HG2	3:D:396:VAL:HG22	1.91	0.52
3:D:1236:LEU:HA	3:J:1359:GLN:HE21	1.73	0.52
2:C:254:LEU:HD12	2:C:257:LEU:HD13	1.91	0.52
2:C:944:LEU:HD22	2:C:962:GLN:HB3	1.90	0.52
2:C:1090:LYS:HA	2:C:1093:GLN:HG3	1.91	0.52
1:B:178:ALA:O	1:B:198:ARG:HB2	2.10	0.52
2:C:474:VAL:O	2:C:474:VAL:HG23	2.10	0.52
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.92	0.52
2:C:988:VAL:HG12	3:D:948:THR:OG1	2.09	0.52
3:D:95:LEU:HG	3:D:574:LEU:HD21	1.92	0.52
1:A:56:VAL:O	1:A:164:ALA:O	2.28	0.52
2:C:607:ASP:O	2:C:609:THR:N	2.42	0.52
3:D:645:PRO:HB3	3:D:723:GLY:O	2.09	0.52
1:A:20:TYR:CD2	1:A:20:TYR:C	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1009:SER:HB3	3:D:651:GLU:O	2.10	0.52
3:D:1219:GLU:O	3:D:1221:VAL:HG23	2.09	0.52
2:C:223:ASP:O	2:C:225:ALA:N	2.38	0.52
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.90	0.52
3:D:804:MET:CG	3:D:805:ALA:H	2.04	0.52
4:K:34:ARG:C	4:K:36:LYS:H	2.07	0.52
1:A:74:ASP:OD2	1:A:76:VAL:HB	2.09	0.52
2:C:198:ARG:NE	2:C:229:MET:O	2.43	0.52
2:C:551:GLU:HG2	2:C:906:PHE:H	1.74	0.52
2:C:1013:TYR:CD1	2:C:1063:ARG:CZ	2.93	0.52
3:D:71:LYS:O	3:D:79:GLU:HA	2.10	0.52
3:D:794:GLN:HB3	3:D:1017:PHE:CZ	2.44	0.52
4:K:40:LEU:HD23	4:K:40:LEU:H	1.74	0.52
2:C:1076:VAL:HG12	2:C:1077:PRO:N	2.24	0.52
3:J:1319:VAL:HG13	3:J:1320:GLU:N	2.25	0.52
1:A:181:VAL:HG12	2:C:938:LYS:HG3	1.91	0.52
1:B:59:GLU:HB3	1:B:139:TYR:HB3	1.91	0.52
2:C:184:MET:CE	2:C:191:PHE:HZ	2.23	0.52
2:C:580:MET:HB3	2:C:584:GLU:CD	2.30	0.52
3:D:665:ALA:O	3:D:666:PHE:C	2.48	0.52
1:A:150:TYR:HD1	1:A:170:ILE:HD13	1.74	0.52
3:D:782:SER:HA	3:D:786:ILE:HD12	1.92	0.52
3:D:813:LEU:CD1	3:D:839:LEU:HD13	2.36	0.52
1:A:30:ARG:HH22	3:D:856:GLY:N	2.04	0.51
3:D:51:GLY:HA3	3:D:85:VAL:HG12	1.91	0.51
3:D:666:PHE:O	3:D:666:PHE:CG	2.63	0.51
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.92	0.51
3:D:647:ARG:NH2	3:D:683:ILE:CD1	2.70	0.51
3:D:483:HIS:N	3:D:484:PRO:HD3	2.25	0.51
3:J:1311:LEU:HA	3:J:1326:THR:HA	1.92	0.51
1:B:11:PHE:HE1	1:B:23:PHE:HB3	1.74	0.51
2:C:203:ASP:OD2	2:C:206:THR:HB	2.10	0.51
2:C:650:LYS:O	2:C:652:GLY:N	2.44	0.51
2:C:751:PRO:HA	2:C:792:VAL:HG12	1.93	0.51
3:D:121:THR:C	3:D:123:LEU:H	2.13	0.51
3:D:858:LEU:HD23	3:D:864:VAL:HG21	1.92	0.51
2:C:24:GLU:O	2:C:28:LYS:HG2	2.11	0.51
2:C:73:ILE:HG13	2:C:94:LEU:CD1	2.39	0.51
2:C:175:GLU:O	2:C:182:VAL:O	2.28	0.51
3:D:699:VAL:H	3:D:756:GLN:HE22	1.53	0.51
3:D:1107:VAL:HG23	3:D:1221:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:LEU:O	2:C:378:LEU:HB3	2.11	0.51
2:C:551:GLU:HG2	2:C:906:PHE:HA	1.93	0.51
2:C:726:ILE:HB	2:C:729:LEU:HD22	1.93	0.51
3:D:609:GLY:HA3	3:D:615:ARG:NH2	2.24	0.51
3:D:1140:ILE:HG21	3:D:1175:ILE:HG12	1.93	0.51
1:B:34:VAL:HG11	2:C:978:ARG:HB3	1.92	0.51
2:C:408:ARG:NH2	2:C:456:ALA:O	2.44	0.51
2:C:841:ASN:ND2	2:C:845:ASN:H	2.08	0.51
2:C:971:LYS:HA	2:C:988:VAL:HA	1.93	0.51
2:C:1015:LEU:HD12	2:C:1015:LEU:H	1.75	0.51
3:D:129:PHE:CZ	3:D:587:ARG:HD2	2.45	0.51
3:D:547:LEU:HD22	3:D:581:VAL:HG21	1.91	0.51
3:J:1256:LEU:HG	3:J:1260:ILE:HD11	1.93	0.51
1:A:65:PHE:HE2	2:C:703:ILE:HG12	1.76	0.51
1:A:170:ILE:HD12	2:C:696:LYS:HB3	1.93	0.51
2:C:64:LEU:HA	2:C:101:ILE:O	2.10	0.51
2:C:333:ILE:HB	2:C:461:VAL:HG11	1.92	0.51
4:K:19:LEU:O	4:K:23:VAL:HG23	2.11	0.51
2:C:431:HIS:CD2	2:C:432:ARG:O	2.64	0.51
2:C:724:ARG:HB2	2:C:741:GLY:HA2	1.93	0.51
2:C:958:SER:O	2:C:962:GLN:N	2.43	0.51
2:C:1088:LEU:CA	3:D:613:ARG:HD3	2.40	0.51
3:D:298:VAL:HG22	3:D:302:GLN:HB3	1.92	0.51
2:C:333:ILE:HD11	2:C:467:ILE:CD1	2.41	0.51
2:C:557:ARG:HD3	2:C:879:ARG:HB3	1.92	0.51
3:D:950:GLY:O	3:D:953:ASP:HB2	2.11	0.51
1:A:9:PRO:HB3	1:A:27:PRO:HD2	1.93	0.50
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.91	0.50
2:C:300:ASP:OD2	2:C:303:PHE:HB2	2.11	0.50
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.46	0.50
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.93	0.50
3:J:1356:TYR:HB3	3:J:1361:VAL:HB	1.93	0.50
1:A:75:VAL:O	1:A:79:ILE:HG13	2.12	0.50
2:C:617:ASP:O	2:C:619:ARG:N	2.39	0.50
3:D:310:LEU:HD23	3:D:310:LEU:H	1.76	0.50
3:D:500:ARG:HA	3:D:503:LEU:HB2	1.93	0.50
3:D:614:PHE:CE1	3:J:1447:LEU:HD11	2.46	0.50
3:D:902:MET:HA	3:D:902:MET:HE2	1.93	0.50
3:D:1060:SER:H	3:D:1063:GLU:HG3	1.76	0.50
3:J:1426:LYS:O	3:J:1429:LEU:HB3	2.11	0.50
1:A:86:VAL:HG13	1:A:124:ASN:OD1	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:THR:HG22	2:C:123:GLU:N	2.25	0.50
2:C:179:SER:HB2	2:C:181:VAL:HG23	1.93	0.50
2:C:979:THR:C	2:C:981:GLU:H	2.14	0.50
2:C:1018:GLN:CG	2:C:1060:ILE:HD11	2.41	0.50
3:J:1453:ALA:O	3:J:1455:LYS:N	2.35	0.50
2:C:261:LEU:CD2	2:C:263:ASP:HB3	2.42	0.50
3:D:648:MET:O	3:D:652:LEU:HB2	2.12	0.50
1:A:62:LEU:HA	1:A:163:ASN:HB3	1.93	0.50
1:B:19:HIS:CD2	1:B:19:HIS:H	2.30	0.50
1:B:30:ARG:HH12	2:C:854:PRO:HG3	1.77	0.50
1:B:54:THR:HG23	1:B:143:ARG:HG2	1.92	0.50
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.92	0.50
2:C:282:GLY:O	2:C:283:VAL:O	2.29	0.50
3:D:224:ARG:HA	3:D:331:VAL:O	2.12	0.50
3:D:556:LYS:O	3:D:557:LEU:C	2.50	0.50
2:C:299:LYS:HG3	2:C:299:LYS:O	2.11	0.50
2:C:537:LYS:HG2	2:C:545:ASN:OD1	2.12	0.50
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.94	0.50
3:D:403:PHE:CE1	3:D:407:VAL:HG22	2.46	0.50
3:D:1129:THR:C	3:D:1131:THR:H	2.15	0.50
3:D:501:ALA:O	3:D:505:SER:HB3	2.11	0.50
1:A:59:GLU:HG2	1:A:139:TYR:HB3	1.93	0.50
1:A:100:ILE:HG23	1:A:139:TYR:CE1	2.46	0.50
2:C:405:ARG:NH1	2:C:566:THR:HG21	2.25	0.50
2:C:685:GLU:HB2	3:D:740:PHE:CD1	2.46	0.50
3:D:111:LYS:HE3	3:J:1449:GLU:HG3	1.93	0.50
2:C:770:GLU:O	2:C:774:LEU:HG	2.11	0.49
3:D:26:VAL:C	3:D:28:LYS:N	2.66	0.49
3:D:415:VAL:HG22	3:D:419:ASP:HB3	1.94	0.49
3:D:926:LYS:NZ	3:D:929:ARG:HH21	2.10	0.49
3:D:1102:ALA:O	3:D:1104:GLU:N	2.45	0.49
1:A:86:VAL:HG22	1:A:86:VAL:O	2.11	0.49
2:C:65:VAL:O	2:C:66:LEU:HB3	2.12	0.49
2:C:72:ARG:HD3	2:C:112:GLU:OE1	2.12	0.49
2:C:351:LEU:O	2:C:355:VAL:HG23	2.13	0.49
3:D:26:VAL:O	3:D:548:ILE:HD13	2.10	0.49
3:D:841:PHE:HB2	3:D:864:VAL:HG22	1.93	0.49
1:A:176:ARG:HG2	1:A:200:TRP:CE3	2.47	0.49
1:A:184:THR:HB	1:A:194:LYS:HB2	1.93	0.49
1:B:189:ARG:CZ	1:B:192:LEU:HD21	2.42	0.49
2:C:141:HIS:HE1	2:C:332:ARG:HH11	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:547:ILE:HG12	2:C:842:ARG:O	2.11	0.49
3:D:176:ASP:HA	3:D:389:GLU:HG2	1.94	0.49
3:D:658:LEU:HD11	3:D:674:ARG:HD2	1.93	0.49
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.93	0.49
3:D:789:LEU:HD12	3:D:911:LEU:HD13	1.94	0.49
3:J:1434:TRP:NE1	3:J:1435:LEU:HD13	2.27	0.49
4:K:16:LYS:O	4:K:19:LEU:HB3	2.13	0.49
5:C:1120:SRN:H421	5:C:1120:SRN:H373	1.94	0.49
3:D:245:LEU:HD11	3:D:311:LEU:HD11	1.93	0.49
2:C:148:PHE:O	2:C:149:THR:CB	2.61	0.49
2:C:810:ASP:HB3	2:C:813:VAL:HG21	1.95	0.49
3:D:87:ARG:HG2	3:D:87:ARG:HH11	1.78	0.49
3:D:119:SER:HB2	3:D:123:LEU:HD13	1.94	0.49
1:A:89:PHE:O	1:A:90:LEU:HB2	2.13	0.49
1:A:160:ASP:O	1:A:161:ARG:HG2	2.12	0.49
2:C:757:GLY:HA2	2:C:789:SER:OG	2.12	0.49
3:J:1336:LEU:HD11	3:J:1419:PRO:HB2	1.94	0.49
2:C:548:PRO:HG3	2:C:842:ARG:NH2	2.28	0.49
3:D:1197:ARG:O	3:D:1199:GLY:N	2.38	0.49
1:B:89:PHE:CB	1:B:146:ARG:HH21	2.25	0.49
1:B:142:VAL:HG22	1:B:142:VAL:O	2.12	0.49
2:C:474:VAL:HG21	2:C:529:VAL:HG12	1.95	0.49
2:C:715:THR:C	2:C:717:LEU:N	2.65	0.49
2:C:929:ARG:HH11	2:C:936:VAL:H	1.61	0.49
3:J:1291:SER:HB3	3:J:1302:GLU:OE1	2.13	0.49
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.95	0.48
2:C:1051:GLU:OE2	3:D:751:LEU:HB2	2.13	0.48
3:D:767:HIS:NE2	4:K:6:ILE:HD12	2.27	0.48
3:D:1109:GLU:OE1	3:D:1196:THR:CG2	2.61	0.48
1:A:110:ARG:O	1:A:110:ARG:HG2	2.13	0.48
2:C:160:ALA:N	2:C:174:LEU:O	2.45	0.48
2:C:508:ILE:HG21	2:C:513:VAL:HG21	1.95	0.48
2:C:575:GLN:NE2	2:C:671:ASN:H	2.10	0.48
2:C:1015:LEU:HD13	3:D:528:VAL:HG11	1.94	0.48
3:D:507:ASN:ND2	3:J:1452:ILE:O	2.46	0.48
3:D:895:VAL:O	3:D:898:GLU:HB3	2.13	0.48
3:D:955:VAL:HG23	3:D:1011:PHE:HE2	1.78	0.48
3:D:1205:TYR:CZ	3:D:1221:VAL:HG13	2.48	0.48
1:A:53:VAL:HG12	1:A:142:VAL:CG2	2.43	0.48
2:C:246:ASP:C	2:C:248:PRO:HD3	2.33	0.48
2:C:999:HIS:C	2:C:1000:MET:HG2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:243:ALA:HB3	3:D:311:LEU:HD12	1.95	0.48
3:D:789:LEU:HD11	3:D:934:LEU:HD22	1.95	0.48
3:D:876:SER:OG	3:D:879:ARG:HG3	2.13	0.48
2:C:79:SER:O	2:C:81:ASP:N	2.47	0.48
2:C:203:ASP:H	2:C:206:THR:HG22	1.78	0.48
3:D:111:LYS:CE	3:J:1449:GLU:HG3	2.43	0.48
3:D:657:LEU:HD23	3:D:677:LEU:HD11	1.95	0.48
3:D:913:ASP:O	3:D:917:GLN:HB2	2.14	0.48
3:D:1208:ASP:C	3:D:1210:SER:N	2.66	0.48
1:A:55:SER:HA	1:A:167:VAL:HG23	1.95	0.48
2:C:13:ILE:HG22	2:C:14:PRO:O	2.14	0.48
2:C:1005:MET:O	2:C:1005:MET:HG3	2.11	0.48
3:D:260:GLU:HB3	3:D:271:TYR:HB2	1.95	0.48
2:C:354:GLY:O	2:C:358:ARG:HG3	2.13	0.48
2:C:1040:LEU:HD23	3:D:713:ILE:HD12	1.96	0.48
3:D:874:GLU:O	3:D:875:THR:O	2.32	0.48
3:D:1221:VAL:HG12	3:J:1370:ILE:HD12	1.95	0.48
2:C:732:ALA:O	2:C:735:ARG:HB2	2.14	0.48
2:C:1009:SER:O	3:D:624:ASP:O	2.32	0.48
3:D:237:ARG:O	3:D:239:GLY:N	2.47	0.48
3:D:637:LEU:HB3	3:D:641:GLN:HB2	1.94	0.48
3:D:806:PHE:O	3:D:833:GLU:HB3	2.13	0.48
3:D:1152:GLU:OE2	3:D:1159:ARG:NH2	2.47	0.48
3:J:1256:LEU:N	3:J:1257:PRO:CD	2.77	0.48
2:C:267:TYR:O	2:C:268:ASP:CB	2.62	0.48
2:C:575:GLN:HE21	2:C:671:ASN:N	2.11	0.48
2:C:680:ASP:OD1	3:D:940:THR:HA	2.14	0.48
3:D:22:SER:O	3:D:90:MET:O	2.32	0.48
4:K:38:THR:HG22	4:K:40:LEU:N	2.29	0.48
1:A:32:PHE:CE2	1:B:221:HIS:CD2	3.02	0.48
1:A:173:PRO:HB3	1:A:205:VAL:HG13	1.95	0.48
3:D:313:LEU:HD11	3:D:319:ALA:HB2	1.96	0.48
3:D:1206:GLY:O	3:D:1207:TYR:HB2	2.14	0.48
4:K:9:LEU:HD23	4:K:12:MET:HE2	1.96	0.48
2:C:922:PHE:CD2	2:C:964:LYS:HD3	2.49	0.47
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.96	0.47
2:C:833:LEU:HD12	2:C:833:LEU:HA	1.64	0.47
2:C:846:LYS:HG3	3:D:741:ASP:HB2	1.95	0.47
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.96	0.47
3:D:1202:GLN:HE22	3:D:1214:PRO:HB2	1.79	0.47
2:C:265:LYS:HE2	2:C:289:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:538:SER:O	3:D:539:ASP:HB3	2.14	0.47
3:D:1207:TYR:H	3:D:1214:PRO:HA	1.79	0.47
3:D:108:VAL:H	3:D:109:PRO:HD2	1.79	0.47
1:B:111:ALA:O	1:B:114:PHE:HD1	1.98	0.47
2:C:489:SER:C	2:C:491:GLU:H	2.18	0.47
2:C:834:GLN:OE1	2:C:1001:VAL:HG23	2.15	0.47
1:A:20:TYR:CE2	1:A:22:GLU:HG3	2.47	0.47
1:A:202:ASP:O	1:A:202:ASP:OD1	2.31	0.47
1:B:79:ILE:HG23	1:B:167:VAL:CG1	2.44	0.47
2:C:54:ILE:O	2:C:65:VAL:O	2.33	0.47
2:C:439:CYS:SG	2:C:441:VAL:O	2.65	0.47
3:D:108:VAL:N	3:D:109:PRO:CD	2.77	0.47
3:D:545:ARG:C	3:D:547:LEU:N	2.66	0.47
3:D:761:ILE:HD13	4:K:20:THR:HA	1.96	0.47
3:D:1237:THR:O	3:J:1255:GLY:HA3	2.15	0.47
2:C:22:GLN:HG2	2:C:125:GLY:O	2.15	0.47
2:C:650:LYS:HB2	2:C:653:ASP:CB	2.44	0.47
3:D:177:ALA:HB1	3:D:393:ILE:HD11	1.97	0.47
2:C:114:PHE:O	2:C:375:SER:HB2	2.15	0.47
2:C:595:LEU:HB3	2:C:656:ALA:HB3	1.97	0.47
3:D:813:LEU:HD11	3:D:839:LEU:HD22	1.97	0.47
3:D:1149:LEU:HD23	3:D:1149:LEU:HA	1.70	0.47
1:A:48:ILE:HD11	1:A:214:ALA:HB2	1.97	0.47
2:C:94:LEU:HD22	2:C:344:PHE:HZ	1.78	0.47
2:C:644:ARG:H	2:C:647:GLN:HE21	1.61	0.47
3:D:84:ILE:O	3:D:87:ARG:HB2	2.15	0.47
2:C:689:VAL:HG11	2:C:870:ILE:HD12	1.96	0.47
3:D:496:LEU:HD23	3:D:500:ARG:HB2	1.96	0.47
3:D:502:PHE:CD2	3:D:509:PRO:HD3	2.50	0.47
2:C:607:ASP:C	2:C:609:THR:H	2.19	0.46
2:C:755:LEU:HG	2:C:792:VAL:HG23	1.96	0.46
2:C:965:GLU:O	2:C:969:LEU:HD13	2.15	0.46
3:D:473:LEU:HD21	3:D:495:ARG:NH1	2.30	0.46
2:C:164:PRO:HB3	2:C:265:LYS:HD2	1.96	0.46
2:C:684:PHE:CE2	2:C:685:GLU:HG2	2.49	0.46
2:C:858:MET:HA	2:C:859:PRO:HD2	1.78	0.46
3:D:167:GLU:O	3:D:394:LEU:HA	2.15	0.46
3:D:892:ASP:OD1	3:D:895:VAL:HG23	2.15	0.46
3:D:1144:LEU:O	3:D:1145:TYR:C	2.53	0.46
1:A:14:THR:O	1:A:14:THR:HG22	2.14	0.46
2:C:375:SER:O	2:C:375:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:432:ARG:HH12	2:C:518:ARG:NH2	2.13	0.46
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.51	0.46
2:C:922:PHE:HB2	2:C:967:PHE:CD2	2.50	0.46
2:C:1095:LEU:O	3:D:101:HIS:HE1	1.98	0.46
3:D:90:MET:HE3	3:D:519:VAL:O	2.16	0.46
3:D:1014:ASN:O	3:D:1015:TYR:CB	2.63	0.46
2:C:26:TYR:O	2:C:27:LYS:C	2.53	0.46
2:C:52:PHE:HB3	2:C:68:PHE:HB3	1.97	0.46
2:C:540:PHE:CE1	2:C:906:PHE:CE1	3.00	0.46
3:D:609:GLY:CA	3:D:615:ARG:HE	2.29	0.46
3:D:1105:ILE:HD12	3:J:1370:ILE:HG23	1.98	0.46
1:A:215:VAL:O	1:A:216:ALA:C	2.53	0.46
3:D:97:THR:CB	3:D:98:PRO:CD	2.74	0.46
3:D:509:PRO:C	3:D:511:TRP:H	2.19	0.46
1:A:55:SER:HB3	1:A:158:ILE:HG13	1.97	0.46
1:B:227:ASN:HA	1:B:228:PRO:HD3	1.78	0.46
2:C:397:GLU:CB	2:C:633:GLN:HE21	2.24	0.46
2:C:462:ASP:CB	2:C:468:ARG:HD2	2.46	0.46
3:D:702:LEU:HB3	3:D:745:MET:HE2	1.97	0.46
2:C:141:HIS:CE1	2:C:332:ARG:HB3	2.51	0.46
2:C:154:ARG:HH12	2:C:157:ARG:HH11	1.64	0.46
2:C:472:ARG:HB3	2:C:532:MET:HB3	1.97	0.46
2:C:1067:TYR:HE1	3:D:655:PRO:HB3	1.81	0.46
3:D:101:HIS:ND1	3:D:514:LEU:HD21	2.30	0.46
3:D:702:LEU:HD23	3:D:747:VAL:HB	1.97	0.46
1:A:140:MET:HE3	1:A:140:MET:HB2	1.87	0.46
1:B:5:LYS:O	1:B:6:LEU:HB3	2.16	0.46
1:B:101:LEU:HD12	1:B:114:PHE:HA	1.98	0.46
2:C:57:GLY:O	2:C:58:ASP:HB2	2.16	0.46
2:C:256:TYR:CE2	2:C:261:LEU:HD22	2.51	0.46
2:C:487:THR:HB	2:C:490:GLU:HB2	1.98	0.46
2:C:678:PRO:HG2	3:D:947:ILE:CD1	2.46	0.46
2:C:730:SER:C	2:C:732:ALA:H	2.19	0.46
3:D:881:LEU:HD12	3:D:881:LEU:O	2.15	0.46
3:D:887:GLY:O	3:D:888:GLU:C	2.53	0.46
3:D:1060:SER:H	3:D:1063:GLU:CG	2.28	0.46
3:D:1220:ALA:O	3:D:1224:VAL:HG23	2.16	0.46
1:A:114:PHE:HZ	1:A:142:VAL:HG11	1.81	0.46
1:A:225:PHE:CE2	1:B:25:LEU:CD2	2.99	0.46
1:B:60:ASP:O	1:B:61:VAL:HB	2.15	0.46
2:C:133:ASP:N	2:C:133:ASP:OD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1173:PHE:CD2	3:D:1173:PHE:C	2.90	0.46
1:B:76:VAL:O	1:B:80:LEU:HG	2.15	0.46
2:C:635:THR:O	2:C:636:ALA:HB3	2.16	0.46
3:D:12:LEU:HA	3:D:12:LEU:HD13	1.82	0.46
3:D:317:MET:HA	3:D:338:GLU:O	2.16	0.46
3:D:666:PHE:O	3:D:667:ALA:HB3	2.16	0.46
3:D:695:ILE:O	3:D:696:HIS:C	2.54	0.46
3:D:921:ARG:CG	3:D:921:ARG:NH1	2.77	0.46
2:C:80:GLN:NE2	2:C:122:THR:HG23	2.28	0.45
2:C:328:LEU:HB2	2:C:433:THR:HG22	1.97	0.45
2:C:863:ASP:OD2	2:C:865:THR:HG23	2.16	0.45
2:C:1030:GLN:NE2	3:D:628:ARG:HB3	2.31	0.45
3:J:1304:LYS:H	3:J:1304:LYS:HZ3	1.64	0.45
3:J:1488:ASP:HB2	4:K:73:LEU:CD2	2.46	0.45
3:D:264:LEU:O	3:D:266:GLU:N	2.49	0.45
3:D:284:LEU:HD13	3:D:305:ALA:HB2	1.98	0.45
3:D:508:ARG:O	3:D:509:PRO:O	2.35	0.45
3:D:646:LYS:HE2	3:D:722:GLU:OE1	2.16	0.45
3:D:842:VAL:HG22	3:D:865:THR:HB	1.97	0.45
3:J:1473:PRO:HA	3:J:1477:GLY:O	2.16	0.45
2:C:141:HIS:HE1	2:C:332:ARG:NH1	2.14	0.45
2:C:606:VAL:HG12	2:C:606:VAL:O	2.17	0.45
3:D:613:ARG:HH22	3:D:616:GLN:HE22	1.64	0.45
3:D:647:ARG:HH22	3:D:683:ILE:HD11	1.78	0.45
3:D:1237:THR:H	3:J:1359:GLN:NE2	2.14	0.45
3:J:1384:PRO:HD3	3:J:1389:LEU:HB2	1.97	0.45
1:B:19:HIS:HA	1:B:201:THR:O	2.16	0.45
1:B:186:LEU:HA	1:B:186:LEU:HD23	1.68	0.45
2:C:8:ARG:HB3	2:C:9:ILE:H	1.64	0.45
2:C:142:ARG:HH11	2:C:142:ARG:CB	2.29	0.45
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.46	0.45
2:C:692:GLU:HG2	2:C:696:LYS:HE2	1.99	0.45
2:C:806:LEU:O	2:C:821:GLU:HA	2.16	0.45
2:C:859:PRO:HD2	2:C:870:ILE:HD11	1.97	0.45
3:D:400:VAL:HG13	3:D:443:VAL:HG21	1.97	0.45
3:J:1327:ARG:HB3	3:J:1328:GLY:H	1.51	0.45
1:A:27:PRO:HG3	1:A:186:LEU:HD13	1.99	0.45
2:C:570:PRO:HD2	2:C:635:THR:HG22	1.97	0.45
3:D:118:LEU:O	3:D:120:ALA:O	2.33	0.45
4:K:35:PHE:H	4:K:35:PHE:HD1	1.63	0.45
1:B:18:ASP:CG	1:B:19:HIS:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:TYR:HB3	1:B:141:GLU:HB2	1.99	0.45
1:B:82:LEU:O	1:B:85:LEU:HB3	2.16	0.45
2:C:901:TYR:HE2	2:C:917:LEU:CD1	2.29	0.45
2:C:937:ASP:OD2	2:C:975:TYR:OH	2.29	0.45
2:C:964:LYS:O	2:C:965:GLU:C	2.54	0.45
3:D:100:ALA:H	3:D:575:GLN:NE2	2.14	0.45
3:D:497:GLU:O	3:D:501:ALA:HB2	2.16	0.45
3:D:551:ASN:OD1	3:D:574:LEU:HD11	2.17	0.45
3:D:702:LEU:CD2	3:D:747:VAL:HB	2.47	0.45
3:D:1191:PRO:HD2	3:J:1369:GLU:OE1	2.17	0.45
3:J:1431:THR:O	3:J:1433:SER:N	2.49	0.45
4:K:26:ARG:C	4:K:28:GLN:N	2.68	0.45
4:K:38:THR:HG1	4:K:63:TRP:HZ3	1.60	0.45
2:C:96:ALA:HB2	2:C:115:LEU:CD1	2.45	0.45
2:C:524:VAL:CG1	2:C:529:VAL:HG23	2.46	0.45
2:C:902:ILE:O	2:C:902:ILE:HG22	2.16	0.45
3:D:936:TYR:C	3:D:936:TYR:CD2	2.90	0.45
3:D:1103:HIS:CE1	3:J:1463:LYS:HB2	2.52	0.45
3:J:1453:ALA:C	3:J:1455:LYS:H	2.19	0.45
1:A:137:LYS:O	1:A:138:LEU:HB2	2.17	0.45
2:C:265:LYS:HG2	2:C:289:THR:OG1	2.16	0.45
2:C:462:ASP:O	2:C:463:ALA:C	2.55	0.45
2:C:841:ASN:C	2:C:841:ASN:ND2	2.62	0.45
3:D:259:VAL:HG12	3:D:272:LEU:HD21	1.99	0.45
1:A:124:ASN:ND2	1:A:127:LEU:HD22	2.32	0.45
3:D:409:VAL:CG1	3:D:435:VAL:HG11	2.41	0.45
3:D:790:TYR:HD1	3:D:906:GLN:O	2.00	0.45
3:D:1202:GLN:NE2	3:D:1214:PRO:HB2	2.32	0.45
1:A:77:GLU:HG3	2:C:640:ARG:CZ	2.47	0.45
1:A:162:ILE:HG22	1:A:163:ASN:H	1.81	0.45
1:B:51:THR:HA	1:B:145:ASP:O	2.16	0.45
3:D:931:LEU:HD12	3:D:931:LEU:HA	1.80	0.45
3:D:1138:SER:O	3:D:1141:GLU:HG3	2.17	0.45
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.98	0.44
2:C:1095:LEU:O	3:D:101:HIS:CE1	2.69	0.44
2:C:1098:ASP:HB3	3:D:11:ALA:HB3	1.98	0.44
3:D:233:LYS:HB2	3:D:236:TYR:CZ	2.52	0.44
3:D:681:ARG:O	3:D:682:ASP:HB2	2.17	0.44
3:D:949:ILE:HG12	3:D:1020:LEU:HD13	1.99	0.44
3:D:1231:GLU:N	3:D:1232:PRO:HD3	2.33	0.44
3:D:154:THR:HB	3:D:157:GLU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:869:LEU:HB3	3:D:870:GLY:H	1.51	0.44
3:D:1140:ILE:HG22	3:D:1144:LEU:HD12	1.99	0.44
2:C:399:ASN:ND2	2:C:399:ASN:C	2.70	0.44
2:C:630:ARG:HG3	2:C:705:ILE:HB	2.00	0.44
2:C:703:ILE:O	2:C:703:ILE:HG22	2.17	0.44
2:C:754:ILE:H	2:C:754:ILE:HG12	1.51	0.44
1:A:143:ARG:HE	1:A:145:ASP:CG	2.21	0.44
1:B:55:SER:HA	1:B:166:PRO:HA	2.00	0.44
1:B:132:LEU:HD22	1:B:132:LEU:H	1.81	0.44
2:C:1018:GLN:HE21	2:C:1063:ARG:HH22	1.64	0.44
2:C:1077:PRO:HB2	2:C:1079:PRO:HD3	1.99	0.44
2:C:191:PHE:HB3	2:C:241:LEU:HD12	2.00	0.44
2:C:839:LEU:HA	2:C:995:MET:O	2.18	0.44
2:C:918:LEU:CD2	2:C:967:PHE:O	2.65	0.44
2:C:984:GLU:HG3	3:D:944:THR:O	2.17	0.44
5:C:1120:SRN:H401	5:C:1120:SRN:C3	2.48	0.44
3:D:36:THR:CG2	3:D:37:LEU:N	2.80	0.44
3:D:450:TYR:CD1	3:D:450:TYR:N	2.86	0.44
3:D:558:LEU:CD2	3:D:567:ILE:HG12	2.47	0.44
3:J:1380:GLU:N	3:J:1420:LEU:HD22	2.33	0.44
2:C:140:ILE:HD11	2:C:331:ARG:NH2	2.32	0.44
2:C:264:PRO:HB2	2:C:265:LYS:H	1.58	0.44
2:C:632:ASN:HB2	2:C:633:GLN:NE2	2.32	0.44
2:C:665:PHE:CD1	2:C:665:PHE:N	2.86	0.44
3:D:56:TYR:O	3:D:57:GLU:O	2.36	0.44
3:D:161:LEU:HB3	3:D:452:ILE:HD11	2.00	0.44
3:D:638:LYS:C	3:D:729:HIS:CD2	2.91	0.44
3:D:653:PHE:CE2	3:D:749:VAL:HG11	2.53	0.44
3:D:792:ILE:HG13	3:D:941:LEU:HG	1.99	0.44
3:D:858:LEU:HD12	3:D:858:LEU:H	1.82	0.44
2:C:148:PHE:CE2	2:C:309:TYR:HB3	2.53	0.44
2:C:230:ARG:O	2:C:233:GLU:N	2.51	0.44
3:D:434:ARG:O	3:D:446:VAL:HA	2.18	0.44
3:D:877:PRO:O	3:D:880:ILE:HB	2.17	0.44
3:D:941:LEU:HD12	3:D:941:LEU:HA	1.76	0.44
4:K:59:ASN:ND2	4:K:61:VAL:CG2	2.71	0.44
2:C:753:ASP:O	2:C:791:ARG:HA	2.16	0.44
2:C:1040:LEU:HD12	2:C:1049:LEU:CA	2.47	0.44
3:D:87:ARG:HG2	3:D:87:ARG:NH1	2.31	0.44
3:D:270:ILE:N	3:D:282:TYR:O	2.48	0.44
1:A:38:ASN:O	1:A:39:PRO:C	2.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:LEU:HD13	2:C:372:LEU:HD11	2.00	0.44
2:C:203:ASP:CG	2:C:206:THR:HB	2.39	0.44
2:C:605:LYS:HB2	2:C:612:ALA:HB3	1.99	0.44
2:C:1046:ALA:HA	3:J:1472:ILE:HG22	2.00	0.44
3:D:434:ARG:HH11	3:D:434:ARG:HB3	1.83	0.44
3:D:629:SER:HB3	3:D:726:ILE:HD12	2.00	0.44
2:C:720:GLU:O	2:C:820:ARG:NH2	2.50	0.43
2:C:1005:MET:HB2	3:D:629:SER:HB2	2.00	0.43
3:D:1221:VAL:HA	3:D:1224:VAL:HG23	1.99	0.43
2:C:400:PRO:HD3	2:C:659:PRO:HG2	1.99	0.43
3:D:783:ARG:HH11	3:D:783:ARG:CG	2.29	0.43
3:D:886:VAL:O	3:D:890:VAL:HB	2.18	0.43
3:J:1434:TRP:CD1	3:J:1434:TRP:C	2.92	0.43
1:B:36:LEU:O	1:B:39:PRO:HD2	2.18	0.43
2:C:7:GLY:HA3	2:C:907:ASP:O	2.18	0.43
2:C:141:HIS:CE1	2:C:332:ARG:NH1	2.85	0.43
2:C:260:LEU:O	2:C:261:LEU:HD23	2.18	0.43
2:C:395:LYS:O	2:C:633:GLN:NE2	2.51	0.43
2:C:562:SER:C	2:C:563:ASN:O	2.55	0.43
3:D:60:CYS:SG	3:D:61:GLY:N	2.90	0.43
3:D:396:VAL:C	3:D:398:ALA:H	2.21	0.43
1:A:61:VAL:CG1	1:A:75:VAL:HG21	2.48	0.43
2:C:70:GLU:HG3	2:C:97:ARG:HG3	2.00	0.43
2:C:247:PRO:N	2:C:248:PRO:HD3	2.34	0.43
2:C:290:LEU:HA	2:C:301:GLU:HB2	1.99	0.43
2:C:564:MET:HG2	2:C:997:LEU:CD1	2.48	0.43
2:C:599:GLU:O	2:C:600:ASP:C	2.56	0.43
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.71	0.43
3:D:545:ARG:O	3:D:546:ARG:C	2.56	0.43
3:D:829:VAL:O	3:D:835:SER:HB3	2.19	0.43
3:D:1076:GLY:C	3:D:1078:ARG:H	2.22	0.43
1:A:57:TYR:O	1:A:140:MET:HA	2.19	0.43
2:C:8:ARG:HA	2:C:8:ARG:HD2	1.62	0.43
2:C:855:VAL:O	2:C:857:ASP:O	2.36	0.43
2:C:890:LEU:O	2:C:893:ALA:HB3	2.19	0.43
3:D:302:GLN:HA	3:D:303:PRO:HD2	1.86	0.43
4:K:39:VAL:HG11	4:K:72:ARG:HB3	2.01	0.43
2:C:600:ASP:HB3	2:C:651:LYS:H	1.84	0.43
2:C:690:ILE:CD1	2:C:869:VAL:HB	2.48	0.43
2:C:859:PRO:O	2:C:867:VAL:HG22	2.18	0.43
2:C:929:ARG:HG2	2:C:934:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1090:LYS:HE3	3:D:88:TYR:O	2.19	0.43
3:D:631:ILE:HD13	3:D:745:MET:SD	2.59	0.43
3:J:1353:GLN:HB3	3:J:1357:ARG:CZ	2.48	0.43
4:K:21:VAL:O	4:K:25:LYS:HB2	2.18	0.43
2:C:34:VAL:HA	2:C:35:PRO:HD3	1.86	0.43
2:C:122:THR:HG22	2:C:123:GLU:H	1.82	0.43
2:C:203:ASP:H	2:C:206:THR:CG2	2.32	0.43
2:C:571:LEU:HD22	2:C:670:GLN:OE1	2.19	0.43
2:C:578:VAL:N	2:C:671:ASN:ND2	2.66	0.43
3:D:789:LEU:HD12	3:D:911:LEU:CD1	2.49	0.43
3:D:875:THR:CG2	3:D:880:ILE:HG12	2.47	0.43
3:D:897:GLN:NE2	3:D:902:MET:SD	2.91	0.43
3:D:1173:PHE:CD2	3:D:1174:LEU:N	2.87	0.43
1:B:39:PRO:O	1:B:43:ILE:HD12	2.19	0.43
1:B:80:LEU:HA	1:B:83:LYS:HD2	2.01	0.43
2:C:36:PRO:HA	2:C:39:ARG:HD2	2.01	0.43
2:C:804:LEU:N	2:C:824:ARG:O	2.51	0.43
3:D:99:ALA:HA	3:D:575:GLN:OE1	2.18	0.43
3:D:896:ALA:O	3:D:900:ILE:HG12	2.19	0.43
3:D:948:THR:O	3:D:1019:PRO:HG3	2.19	0.43
3:D:1065:LEU:HD13	3:D:1069:GLU:HB2	2.01	0.43
3:J:1382:THR:O	3:J:1416:ALA:HB3	2.19	0.43
4:K:38:THR:HG23	4:K:40:LEU:HD23	1.99	0.43
1:A:150:TYR:HD1	1:A:170:ILE:CD1	2.32	0.43
2:C:517:ARG:NH2	2:C:528:GLU:OE2	2.52	0.43
2:C:690:ILE:HD12	2:C:690:ILE:HA	1.71	0.43
2:C:807:ARG:O	2:C:810:ASP:HB2	2.19	0.43
2:C:810:ASP:HB3	2:C:813:VAL:HG23	2.01	0.43
2:C:1011:GLY:HA3	2:C:1012:PRO:HD3	1.78	0.43
3:D:767:HIS:CE1	4:K:3:GLU:HB2	2.54	0.43
3:D:955:VAL:HG23	3:D:1011:PHE:CE2	2.54	0.43
4:K:31:LEU:HD12	4:K:31:LEU:HA	1.61	0.43
2:C:184:MET:HE3	2:C:191:PHE:CZ	2.44	0.43
3:D:18:ILE:HD13	3:D:518:PRO:HD3	2.00	0.43
3:D:455:ARG:HH21	3:D:463:GLU:HG3	1.83	0.43
3:D:756:GLN:O	3:D:760:ARG:HG2	2.19	0.43
3:D:846:PRO:HB3	3:D:880:ILE:CG2	2.49	0.43
3:J:1260:ILE:HG12	3:J:1260:ILE:H	1.58	0.43
2:C:356:ARG:HA	2:C:359:MET:HG3	2.01	0.42
2:C:606:VAL:HG22	2:C:611:ILE:HG12	2.01	0.42
2:C:1094:ALA:HB1	3:D:603:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:591:VAL:O	3:D:600:LEU:HG	2.19	0.42
3:D:1102:ALA:HB1	3:D:1222:GLY:CA	2.49	0.42
3:J:1294:VAL:HG12	3:J:1294:VAL:O	2.19	0.42
3:J:1331:ASP:HB3	3:J:1334:GLN:HB2	2.01	0.42
3:J:1399:ASP:C	3:J:1401:GLU:H	2.21	0.42
4:K:41:GLU:O	4:K:42:PRO:C	2.56	0.42
1:A:125:PRO:O	1:A:126:ASP:HB2	2.19	0.42
2:C:563:ASN:C	2:C:565:GLN:H	2.22	0.42
2:C:810:ASP:HA	2:C:811:PRO:HD2	1.81	0.42
2:C:1043:TYR:CE2	3:D:710:ARG:HD3	2.53	0.42
3:D:141:VAL:HA	3:D:450:TYR:CD2	2.54	0.42
3:D:553:ARG:C	3:D:555:LYS:H	2.23	0.42
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.53	0.42
3:J:1269:LYS:O	3:J:1270:ALA:HB3	2.19	0.42
1:A:73:GLU:H	1:A:73:GLU:HG2	1.36	0.42
1:A:111:ALA:H	1:A:129:ILE:HG13	1.83	0.42
1:B:165:ILE:HA	1:B:166:PRO:HD3	1.91	0.42
2:C:21:ILE:H	2:C:21:ILE:HG13	1.47	0.42
2:C:28:LYS:HG2	2:C:28:LYS:H	1.67	0.42
2:C:154:ARG:HH22	2:C:157:ARG:HH12	1.65	0.42
2:C:433:THR:HG23	2:C:488:ALA:HB1	2.00	0.42
2:C:749:VAL:HG11	2:C:755:LEU:HD21	2.01	0.42
3:J:1417:TRP:CD1	3:J:1417:TRP:C	2.92	0.42
3:J:1432:LYS:O	3:J:1455:LYS:NZ	2.50	0.42
1:A:44:LEU:HA	1:A:48:ILE:HD12	2.01	0.42
2:C:41:ASN:HB3	2:C:42:VAL:H	1.61	0.42
2:C:144:PRO:HG3	2:C:165:LEU:HG	2.01	0.42
2:C:184:MET:CE	2:C:191:PHE:CZ	3.03	0.42
3:D:1213:ARG:HB3	3:D:1214:PRO:HD2	2.01	0.42
4:K:6:ILE:HA	4:K:9:LEU:HD12	2.02	0.42
4:K:33:HIS:O	4:K:34:ARG:C	2.56	0.42
1:A:18:ASP:O	1:A:207:PRO:HD2	2.19	0.42
1:B:91:ASP:HA	1:B:92:PRO:HD3	1.87	0.42
2:C:22:GLN:HG3	2:C:336:VAL:HG21	2.01	0.42
2:C:118:LEU:HD12	2:C:119:PRO:HD2	2.00	0.42
2:C:501:THR:HA	2:C:502:PRO:HD3	1.89	0.42
3:D:805:ALA:HB3	3:D:831:GLY:HA3	2.01	0.42
4:K:39:VAL:HG12	4:K:72:ARG:HD2	2.01	0.42
1:A:58:ILE:HG12	1:A:140:MET:HG3	2.02	0.42
1:B:89:PHE:HB2	1:B:146:ARG:HH21	1.84	0.42
1:B:150:TYR:HD1	1:B:170:ILE:CG2	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:HA	1:B:217:ILE:HD12	2.02	0.42
2:C:35:PRO:HA	2:C:36:PRO:HD3	1.83	0.42
2:C:363:SER:HA	2:C:364:PRO:HD3	1.81	0.42
2:C:399:ASN:HD22	2:C:401:LEU:N	2.16	0.42
2:C:575:GLN:CG	2:C:670:GLN:HG3	2.49	0.42
2:C:841:ASN:ND2	2:C:843:HIS:H	2.18	0.42
3:D:550:ARG:HH22	3:D:553:ARG:HH11	1.66	0.42
3:D:646:LYS:HB2	3:D:688:TRP:CH2	2.55	0.42
3:D:794:GLN:HB3	3:D:1017:PHE:CE2	2.55	0.42
2:C:257:LEU:C	2:C:264:PRO:HG2	2.40	0.42
2:C:336:VAL:O	2:C:337:GLY:C	2.58	0.42
2:C:894:GLY:O	2:C:898:GLY:N	2.50	0.42
3:D:651:GLU:O	3:D:652:LEU:C	2.57	0.42
1:A:192:LEU:O	2:C:938:LYS:NZ	2.53	0.42
2:C:75:ASP:HA	2:C:76:PRO:HD3	1.89	0.42
2:C:564:MET:CE	2:C:846:LYS:HB3	2.50	0.42
3:D:36:THR:CG2	3:D:37:LEU:H	2.26	0.42
3:D:909:ASN:O	3:D:910:SER:C	2.58	0.42
3:D:911:LEU:O	3:D:915:VAL:HG23	2.20	0.42
3:D:951:ILE:C	3:D:953:ASP:H	2.23	0.42
3:D:955:VAL:CG2	3:D:1011:PHE:HE2	2.33	0.42
3:D:1102:ALA:O	3:D:1103:HIS:C	2.58	0.42
3:J:1363:LEU:HD12	3:J:1364:HIS:O	2.20	0.42
2:C:520:GLU:HA	2:C:521:PRO:HD3	1.96	0.42
2:C:745:ILE:CG2	2:C:746:GLY:N	2.83	0.42
2:C:762:LYS:CD	2:C:786:LYS:HD3	2.45	0.42
2:C:1027:PHE:H	2:C:1027:PHE:HD2	1.67	0.42
2:C:1051:GLU:OE2	3:D:752:SER:OG	2.33	0.42
3:D:711:LEU:HB3	3:D:735:ALA:HB1	2.02	0.42
3:D:907:GLU:O	3:D:908:LYS:C	2.57	0.42
3:D:1124:GLN:O	3:D:1132:LEU:HA	2.20	0.42
3:J:1491:THR:O	3:J:1495:ILE:HB	2.19	0.42
1:B:54:THR:HG21	1:B:145:ASP:OD1	2.20	0.42
2:C:292:ARG:HA	2:C:298:PHE:HA	2.02	0.42
2:C:541:SER:OG	2:C:542:LEU:N	2.53	0.42
2:C:564:MET:SD	2:C:846:LYS:HB3	2.59	0.42
2:C:637:PHE:HA	2:C:659:PRO:HB3	2.01	0.42
3:D:798:GLU:OE2	3:D:828:VAL:HG23	2.19	0.42
3:D:860:LEU:HA	3:D:877:PRO:HG2	2.01	0.42
3:D:1156:LEU:HD23	3:D:1182:GLU:OE1	2.20	0.42
3:J:1400:VAL:HG12	3:J:1400:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ILE:O	1:A:71:VAL:HB	2.20	0.41
1:A:122:ILE:HG22	1:A:125:PRO:HD3	2.01	0.41
1:B:18:ASP:CG	1:B:19:HIS:N	2.73	0.41
1:B:104:GLU:HG3	1:B:105:GLY:H	1.84	0.41
2:C:140:ILE:CG2	2:C:333:ILE:HG12	2.50	0.41
3:D:139:GLY:HA2	3:D:452:ILE:CG2	2.43	0.41
3:D:348:ALA:O	3:D:349:PRO:C	2.59	0.41
3:D:678:GLU:O	3:D:680:GLN:N	2.54	0.41
3:D:777:PRO:CG	3:D:912:LYS:HG3	2.47	0.41
3:D:1014:ASN:O	3:D:1015:TYR:CG	2.72	0.41
3:D:1103:HIS:CG	3:D:1104:GLU:N	2.88	0.41
3:J:1452:ILE:HG22	3:J:1453:ALA:N	2.35	0.41
2:C:254:LEU:O	2:C:257:LEU:HB2	2.20	0.41
2:C:689:VAL:HB	2:C:870:ILE:HB	2.02	0.41
3:D:9:ARG:HG3	3:J:1454:GLY:O	2.19	0.41
3:D:100:ALA:H	3:D:575:GLN:CD	2.22	0.41
3:D:112:ILE:C	3:D:114:THR:H	2.23	0.41
3:D:272:LEU:HD12	3:D:282:TYR:HE1	1.85	0.41
2:C:215:GLY:HA3	2:C:217:LEU:HG	2.02	0.41
2:C:551:GLU:HG2	2:C:906:PHE:N	2.35	0.41
2:C:745:ILE:HA	2:C:800:VAL:HG12	2.02	0.41
3:D:614:PHE:HE1	3:J:1447:LEU:HD11	1.84	0.41
3:D:1111:ASP:HB2	3:D:1203:LYS:HD2	2.02	0.41
3:J:1256:LEU:N	3:J:1257:PRO:HD2	2.35	0.41
4:K:45:ARG:NH1	4:K:56:ASP:OD2	2.53	0.41
1:A:49:PRO:HB3	1:A:148:VAL:HG22	2.01	0.41
1:A:172:SER:HA	1:A:173:PRO:HD2	1.82	0.41
1:B:151:VAL:HG23	1:B:171:PHE:HE1	1.86	0.41
1:B:224:TYR:C	1:B:226:ALA:H	2.22	0.41
2:C:549:PHE:CZ	2:C:909:ALA:HB3	2.55	0.41
3:D:118:LEU:O	3:D:119:SER:C	2.58	0.41
3:J:1290:LEU:HD21	3:J:1311:LEU:HD22	2.02	0.41
1:A:111:ALA:O	1:A:114:PHE:HD1	2.03	0.41
1:A:125:PRO:O	1:A:126:ASP:CB	2.68	0.41
1:A:206:THR:HG22	1:A:208:LEU:N	2.28	0.41
2:C:15:LEU:HB2	2:C:586:ARG:NH1	2.36	0.41
2:C:290:LEU:HD12	2:C:291:VAL:N	2.36	0.41
2:C:437:ARG:HB3	2:C:467:ILE:HB	2.02	0.41
2:C:577:PRO:HB3	2:C:993:PHE:CD2	2.56	0.41
2:C:644:ARG:HH11	2:C:645:VAL:HG23	1.86	0.41
2:C:1033:GLY:N	2:C:1036:GLU:OE1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1067:TYR:CE1	3:D:655:PRO:HB3	2.55	0.41
2:C:1088:LEU:HD12	3:D:613:ARG:CG	2.51	0.41
3:D:28:LYS:HB2	3:D:42:ASP:O	2.20	0.41
3:D:47:GLU:HG2	3:D:53:ILE:H	1.85	0.41
3:D:110:SER:O	3:D:112:ILE:N	2.54	0.41
3:D:519:VAL:HA	3:D:544:TYR:CZ	2.55	0.41
3:D:1221:VAL:HG23	3:D:1221:VAL:H	1.64	0.41
1:A:35:THR:HG23	1:B:42:ARG:HD3	2.02	0.41
2:C:256:TYR:CD2	2:C:261:LEU:HD22	2.56	0.41
2:C:469:THR:O	2:C:485:TYR:HA	2.20	0.41
2:C:551:GLU:HG2	2:C:906:PHE:CA	2.49	0.41
2:C:948:GLU:C	2:C:950:LEU:N	2.74	0.41
3:D:100:ALA:H	3:D:575:GLN:HE22	1.67	0.41
3:D:647:ARG:HH21	3:D:683:ILE:CD1	2.33	0.41
3:J:1264:GLU:OE2	3:J:1425:THR:CB	2.68	0.41
3:J:1271:LYS:HG2	3:J:1331:ASP:HB2	2.01	0.41
1:A:23:PHE:CE2	1:A:199:ILE:HD12	2.56	0.41
1:A:111:ALA:O	1:A:114:PHE:N	2.50	0.41
1:A:178:ALA:HB2	2:C:864:GLY:CA	2.51	0.41
2:C:159:ILE:HG22	2:C:175:GLU:CB	2.46	0.41
2:C:277:ALA:O	2:C:281:LEU:CB	2.69	0.41
3:D:14:SER:O	3:D:17:LYS:N	2.42	0.41
3:D:1204:CYS:O	3:D:1206:GLY:N	2.53	0.41
2:C:176:VAL:HG23	2:C:180:GLY:O	2.20	0.41
2:C:185:LYS:NZ	2:C:188:LYS:HA	2.35	0.41
2:C:328:LEU:H	2:C:433:THR:HG21	1.85	0.41
2:C:397:GLU:HB2	2:C:633:GLN:NE2	2.26	0.41
2:C:487:THR:CG2	2:C:488:ALA:N	2.84	0.41
2:C:1006:HIS:HA	2:C:1027:PHE:CZ	2.56	0.41
2:C:1054:THR:OG1	2:C:1055:ILE:N	2.54	0.41
3:D:85:VAL:HG13	3:D:89:ARG:CD	2.51	0.41
3:D:1124:GLN:O	3:D:1124:GLN:HG3	2.20	0.41
1:A:79:ILE:HA	1:A:82:LEU:HD12	2.02	0.41
1:A:87:VAL:HG11	1:A:144:VAL:HG11	2.02	0.41
2:C:198:ARG:CZ	2:C:229:MET:O	2.68	0.41
2:C:246:ASP:HA	2:C:247:PRO:HD3	1.73	0.41
2:C:250:LYS:H	2:C:250:LYS:HG2	1.64	0.41
2:C:261:LEU:HG	2:C:263:ASP:N	2.30	0.41
2:C:340:MET:SD	2:C:340:MET:C	2.99	0.41
2:C:397:GLU:O	2:C:398:THR:C	2.58	0.41
2:C:701:THR:HG22	2:C:832:LYS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:995:MET:HE2	2:C:995:MET:HB2	1.79	0.41
3:D:371:ILE:H	3:D:371:ILE:HG13	1.56	0.41
3:D:642:CYS:SG	3:D:702:LEU:HD11	2.60	0.41
3:D:771:SER:HA	3:D:772:PRO:HD3	1.74	0.41
3:D:907:GLU:HB2	3:D:1026:SER:HA	2.02	0.41
3:D:1037:GLN:NE2	3:D:1042:ARG:HE	2.14	0.41
3:D:1211:MET:H	3:D:1211:MET:HG2	1.73	0.41
3:J:1453:ALA:C	3:J:1455:LYS:N	2.75	0.41
1:A:87:VAL:O	1:A:87:VAL:HG23	2.21	0.41
1:B:179:PHE:CD1	1:B:179:PHE:O	2.73	0.41
2:C:254:LEU:HG	2:C:258:PHE:CE1	2.54	0.41
2:C:264:PRO:O	2:C:266:ARG:N	2.54	0.41
2:C:702:SER:O	2:C:831:ARG:N	2.53	0.41
3:D:101:HIS:HB3	3:D:104:PHE:CD1	2.53	0.41
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.03	0.41
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.56	0.41
3:D:654:LYS:N	3:D:655:PRO:HD2	2.35	0.41
3:D:721:VAL:HG21	3:D:727:GLN:HE22	1.84	0.41
3:J:1448:THR:HG22	3:J:1449:GLU:N	2.36	0.41
2:C:30:LEU:O	2:C:32:ALA:N	2.47	0.40
2:C:451:LEU:HD23	2:C:451:LEU:HA	1.87	0.40
2:C:762:LYS:HB3	2:C:764:GLU:OE2	2.21	0.40
3:D:790:TYR:CD2	3:D:1022:VAL:HG13	2.56	0.40
3:D:882:PHE:HA	3:D:885:ILE:HD12	2.03	0.40
4:K:19:LEU:O	4:K:20:THR:C	2.59	0.40
4:K:40:LEU:CD2	4:K:67:GLU:HG3	2.50	0.40
1:A:38:ASN:OD1	2:C:980:GLY:N	2.54	0.40
1:A:229:GLU:HG2	1:A:230:ALA:H	1.86	0.40
2:C:67:ASP:N	2:C:99:GLN:O	2.46	0.40
2:C:164:PRO:HB3	2:C:265:LYS:HD3	1.99	0.40
2:C:395:LYS:HG2	2:C:397:GLU:HG3	2.02	0.40
2:C:472:ARG:O	2:C:532:MET:N	2.53	0.40
2:C:1013:TYR:CE2	3:D:624:ASP:OD2	2.74	0.40
3:D:121:THR:C	3:D:123:LEU:N	2.73	0.40
3:D:920:LEU:HA	3:D:920:LEU:HD23	1.66	0.40
3:D:1105:ILE:HG21	3:J:1370:ILE:HD13	2.02	0.40
3:D:1205:TYR:O	3:D:1206:GLY:O	2.39	0.40
3:D:1209:LEU:HB3	3:D:1211:MET:HG2	2.03	0.40
1:A:133:GLU:O	1:A:134:GLU:C	2.60	0.40
2:C:21:ILE:HD11	2:C:408:ARG:HG2	2.03	0.40
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:LEU:HB3	2:C:369:PRO:HD3	2.02	0.40
2:C:607:ASP:C	2:C:609:THR:N	2.75	0.40
2:C:642:ARG:HD3	2:C:642:ARG:HA	1.65	0.40
2:C:700:TYR:HB3	2:C:833:LEU:HD22	2.03	0.40
2:C:754:ILE:HD13	2:C:791:ARG:CZ	2.51	0.40
2:C:1100:GLN:OE1	2:C:1102:LEU:HD21	2.21	0.40
3:D:827:ILE:H	3:D:827:ILE:HG12	1.75	0.40
2:C:101:ILE:H	2:C:101:ILE:HG12	1.66	0.40
2:C:151:ASP:HA	2:C:152:PRO:HD3	1.82	0.40
2:C:540:PHE:HB3	2:C:544:THR:HB	2.02	0.40
2:C:755:LEU:CB	2:C:790:LEU:HD23	2.51	0.40
3:D:17:LYS:O	3:D:20:SER:N	2.54	0.40
3:D:314:PRO:HD2	3:D:317:MET:HB2	2.02	0.40
3:J:1262:LEU:HD12	3:J:1348:LEU:HD12	2.04	0.40
1:A:99:LEU:HD21	1:A:120:VAL:HG11	2.04	0.40
2:C:437:ARG:HD3	2:C:467:ILE:O	2.22	0.40
2:C:584:GLU:H	2:C:584:GLU:HG2	1.53	0.40
2:C:838:LYS:HE3	3:D:741:ASP:O	2.21	0.40
2:C:881:ASN:ND2	2:C:881:ASN:N	2.25	0.40
3:D:28:LYS:O	3:D:29:PRO:O	2.40	0.40
3:D:609:GLY:HA3	3:D:615:ARG:HE	1.87	0.40
3:D:923:GLY:O	3:D:925:GLU:N	2.54	0.40
3:D:1076:GLY:O	3:D:1079:LYS:HG2	2.21	0.40
3:J:1347:TYR:CZ	3:J:1351:GLU:HG3	2.56	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	228/314 (73%)	169 (74%)	45 (20%)	14 (6%)	1 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	223/314 (71%)	177 (79%)	33 (15%)	13 (6%)	1 13
2	C	1112/1119 (99%)	859 (77%)	168 (15%)	85 (8%)	1 7
3	D	1236/1524 (81%)	971 (79%)	186 (15%)	79 (6%)	1 10
3	J	247/1524 (16%)	190 (77%)	39 (16%)	18 (7%)	1 7
4	K	93/99 (94%)	66 (71%)	18 (19%)	9 (10%)	0 3
All	All	3139/4894 (64%)	2432 (78%)	489 (16%)	218 (7%)	1 8

All (218) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	A	111	ALA
1	A	139	TYR
1	A	187	GLY
1	A	203	GLY
1	B	26	GLU
1	B	117	SER
1	B	129	ILE
2	C	9	ILE
2	C	38	LYS
2	C	42	VAL
2	C	80	GLN
2	C	132	ALA
2	C	183	THR
2	C	223	ASP
2	C	264	PRO
2	C	265	LYS
2	C	267	TYR
2	C	268	ASP
2	C	283	VAL
2	C	293	PHE
2	C	394	PHE
2	C	463	ALA
2	C	618	GLY
2	C	762	LYS
2	C	769	PRO
2	C	810	ASP
2	C	811	PRO
2	C	821	GLU
2	C	1076	VAL

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Mol	Chain	Res	Type
2	C	1077	PRO
3	D	29	PRO
3	D	32	ILE
3	D	57	GLU
3	D	82	ARG
3	D	97	THR
3	D	98	PRO
3	D	107	ASP
3	D	108	VAL
3	D	136	ASP
3	D	238	PRO
3	D	265	ALA
3	D	300	VAL
3	D	667	ALA
3	D	679	ARG
3	D	680	GLN
3	D	705	ALA
3	D	783	ARG
3	D	827	ILE
3	D	875	THR
3	D	924	MET
3	D	1015	TYR
3	D	1061	PHE
3	D	1067	VAL
3	D	1208	ASP
3	J	1272	ALA
3	J	1327	ARG
3	J	1432	LYS
3	J	1441	GLN
3	J	1489	GLN
4	K	2	ALA
4	K	35	PHE
4	K	41	GLU
4	K	42	PRO
1	A	90	LEU
1	A	138	LEU
1	A	230	ALA
1	B	6	LEU
1	B	61	VAL
1	B	126	ASP
1	B	204	SER
2	C	17	PRO

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Mol	Chain	Res	Type
2	C	64	LEU
2	C	111	ASP
2	C	112	GLU
2	C	315	ALA
2	C	316	GLY
2	C	370	ALA
2	C	416	GLY
2	C	433	THR
2	C	442	GLU
2	C	608	GLY
2	C	636	ALA
2	C	651	LYS
2	C	716	LYS
2	C	980	GLY
3	D	44	LEU
3	D	119	SER
3	D	132	TYR
3	D	150	ARG
3	D	152	LEU
3	D	228	SER
3	D	448	GLU
3	D	509	PRO
3	D	546	ARG
3	D	594	PRO
3	D	600	LEU
3	D	610	LYS
3	D	613	ARG
3	D	696	HIS
3	D	775	GLY
3	D	784	ASP
3	D	800	LYS
3	D	804	MET
3	D	980	MET
3	D	1197	ARG
3	D	1206	GLY
3	J	1307	LYS
3	J	1328	GLY
4	K	52	GLU
1	A	7	LYS
1	A	191	ASP
1	B	20	TYR
2	C	29	ALA

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Mol	Chain	Res	Type
2	C	148	PHE
2	C	270	GLY
2	C	284	GLY
2	C	336	VAL
2	C	418	LEU
2	C	519	GLY
2	C	600	ASP
2	C	740	GLU
2	C	770	GLU
2	C	788	THR
2	C	907	ASP
2	C	945	ALA
2	C	1059	ASP
3	D	34	TYR
3	D	69	GLU
3	D	111	LYS
3	D	181	ASP
3	D	184	GLU
3	D	487	ALA
3	D	539	ASP
3	D	554	LEU
3	D	1028	ALA
3	D	1103	HIS
3	D	1207	TYR
3	J	1299	PHE
3	J	1360	GLY
3	J	1464	GLU
4	K	36	LYS
4	K	87	LYS
4	K	94	PRO
1	A	127	LEU
1	A	199	ILE
1	B	60	ASP
1	B	63	HIS
1	B	127	LEU
2	C	18	LEU
2	C	41	ASN
2	C	213	ALA
2	C	247	PRO
2	C	287	GLY
2	C	295	ASP
2	C	417	GLY

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Mol	Chain	Res	Type
2	C	475	LYS
2	C	490	GLU
2	C	551	GLU
2	C	685	GLU
2	C	700	TYR
2	C	858	MET
3	D	194	GLY
3	D	328	GLY
3	D	795	VAL
3	D	1077	ALA
3	D	1091	SER
3	D	1111	ASP
3	D	1127	GLU
3	D	1137	ARG
3	D	1239	ARG
3	J	1321	ALA
4	K	80	VAL
1	A	27	PRO
1	A	112	GLY
1	B	18	ASP
1	B	154	GLU
2	C	87	ASP
2	C	222	LEU
2	C	312	ALA
2	C	422	ARG
2	C	616	GLU
2	C	699	PHE
2	C	1111	ILE
3	D	117	ASP
3	D	154	THR
3	D	207	PHE
3	D	246	SER
3	D	349	PRO
3	D	584	ASN
3	D	621	LYS
3	D	666	PHE
3	D	981	GLY
3	J	1267	ARG
3	J	1407	LEU
3	J	1412	LYS
3	J	1415	VAL
3	J	1458	GLU

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Mol	Chain	Res	Type
2	C	8	ARG
2	C	11	GLU
2	C	106	GLY
2	C	224	GLU
2	C	376	ARG
2	C	518	ARG
2	C	731	GLU
2	C	1028	GLY
2	C	1099	VAL
3	D	27	GLU
3	D	629	SER
3	D	828	VAL
3	J	1383	ASP
3	D	139	GLY
2	C	36	PRO
2	C	936	VAL
2	C	52	PHE
2	C	263	ASP
3	D	285	PRO
3	J	1454	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	189/270 (70%)	135 (71%)	54 (29%)	0 1
1	B	191/270 (71%)	138 (72%)	53 (28%)	0 1
2	C	889/936 (95%)	633 (71%)	256 (29%)	0 1
3	D	992/1281 (77%)	715 (72%)	277 (28%)	0 1
3	J	191/1281 (15%)	123 (64%)	68 (36%)	0 0
4	K	75/88 (85%)	53 (71%)	22 (29%)	0 1
All	All	2527/4126 (61%)	1797 (71%)	730 (29%)	0 1

All (730) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	12	THR
1	A	15	THR
1	A	18	ASP
1	A	20	TYR
1	A	30	ARG
1	A	38	ASN
1	A	40	LEU
1	A	55	SER
1	A	56	VAL
1	A	59	GLU
1	A	62	LEU
1	A	66	SER
1	A	68	ILE
1	A	72	LYS
1	A	73	GLU
1	A	77	GLU
1	A	85	LEU
1	A	86	VAL
1	A	89	PHE
1	A	94	MET
1	A	101	LEU
1	A	102	ARG
1	A	107	LYS
1	A	110	ARG
1	A	117	SER
1	A	119	ASP
1	A	121	GLU
1	A	127	LEU
1	A	131	THR
1	A	133	GLU
1	A	134	GLU
1	A	138	LEU
1	A	140	MET
1	A	142	VAL
1	A	159	LYS
1	A	161	ARG
1	A	162	ILE
1	A	163	ASN
1	A	165	ILE
1	A	175	ARG
1	A	176	ARG
1	A	183	ASP

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Mol	Chain	Res	Type
1	A	186	LEU
1	A	190	THR
1	A	191	ASP
1	A	195	LEU
1	A	196	THR
1	A	197	LEU
1	A	198	ARG
1	A	208	LEU
1	A	215	VAL
1	A	222	LEU
1	A	231	SER
1	B	7	LYS
1	B	12	THR
1	B	15	THR
1	B	19	HIS
1	B	25	LEU
1	B	34	VAL
1	B	40	LEU
1	B	44	LEU
1	B	47	SER
1	B	55	SER
1	B	56	VAL
1	B	61	VAL
1	B	66	SER
1	B	67	THR
1	B	74	ASP
1	B	75	VAL
1	B	76	VAL
1	B	81	ASN
1	B	82	LEU
1	B	87	VAL
1	B	96	SER
1	B	99	LEU
1	B	100	ILE
1	B	104	GLU
1	B	107	LYS
1	B	109	VAL
1	B	119	ASP
1	B	120	VAL
1	B	126	ASP
1	B	132	LEU
1	B	138	LEU

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Mol	Chain	Res	Type
1	B	142	VAL
1	B	145	ASP
1	B	146	ARG
1	B	148	VAL
1	B	159	LYS
1	B	160	ASP
1	B	161	ARG
1	B	170	ILE
1	B	171	PHE
1	B	172	SER
1	B	174	VAL
1	B	175	ARG
1	B	179	PHE
1	B	180	GLN
1	B	182	GLU
1	B	183	ASP
1	B	186	LEU
1	B	194	LYS
1	B	195	LEU
1	B	197	LEU
1	B	202	ASP
1	B	213	GLN
2	C	4	LYS
2	C	8	ARG
2	C	9	ILE
2	C	10	ARG
2	C	21	ILE
2	C	22	GLN
2	C	23	VAL
2	C	26	TYR
2	C	28	LYS
2	C	30	LEU
2	C	31	GLN
2	C	34	VAL
2	C	42	VAL
2	C	45	GLN
2	C	50	GLU
2	C	51	THR
2	C	52	PHE
2	C	54	ILE
2	C	56	GLU
2	C	61	LYS

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Mol	Chain	Res	Type
2	C	70	GLU
2	C	73	ILE
2	C	75	ASP
2	C	86	LYS
2	C	87	ASP
2	C	94	LEU
2	C	97	ARG
2	C	100	LEU
2	C	101	ILE
2	C	103	LYS
2	C	109	LYS
2	C	110	GLU
2	C	111	ASP
2	C	112	GLU
2	C	113	VAL
2	C	129	ILE
2	C	133	ASP
2	C	138	SER
2	C	142	ARG
2	C	146	VAL
2	C	161	SER
2	C	172	ILE
2	C	176	VAL
2	C	177	GLU
2	C	179	SER
2	C	184	MET
2	C	185	LYS
2	C	186	VAL
2	C	193	LEU
2	C	194	VAL
2	C	195	LEU
2	C	198	ARG
2	C	200	LEU
2	C	204	GLN
2	C	207	LEU
2	C	208	VAL
2	C	214	TYR
2	C	218	VAL
2	C	219	GLN
2	C	223	ASP
2	C	227	LEU
2	C	229	MET

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Mol	Chain	Res	Type
2	C	232	GLU
2	C	233	GLU
2	C	237	ARG
2	C	240	THR
2	C	241	LEU
2	C	242	LEU
2	C	243	ARG
2	C	246	ASP
2	C	250	LYS
2	C	252	LYS
2	C	257	LEU
2	C	258	PHE
2	C	261	LEU
2	C	265	LYS
2	C	275	TYR
2	C	283	VAL
2	C	290	LEU
2	C	293	PHE
2	C	295	ASP
2	C	301	GLU
2	C	322	VAL
2	C	332	ARG
2	C	335	THR
2	C	336	VAL
2	C	343	GLN
2	C	344	PHE
2	C	346	VAL
2	C	348	LEU
2	C	353	ARG
2	C	365	ASP
2	C	366	THR
2	C	371	LYS
2	C	375	SER
2	C	388	ARG
2	C	391	LEU
2	C	394	PHE
2	C	399	ASN
2	C	405	ARG
2	C	406	HIS
2	C	408	ARG
2	C	409	ARG
2	C	413	LEU

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Mol	Chain	Res	Type
2	C	419	THR
2	C	432	ARG
2	C	441	VAL
2	C	445	GLU
2	C	448	ASN
2	C	449	ILE
2	C	454	SER
2	C	460	ARG
2	C	462	ASP
2	C	467	ILE
2	C	472	ARG
2	C	475	LYS
2	C	478	VAL
2	C	495	THR
2	C	498	GLN
2	C	504	GLU
2	C	514	VAL
2	C	523	ILE
2	C	529	VAL
2	C	530	GLU
2	C	541	SER
2	C	542	LEU
2	C	543	ASN
2	C	544	THR
2	C	545	ASN
2	C	551	GLU
2	C	556	ASN
2	C	557	ARG
2	C	559	LEU
2	C	563	ASN
2	C	566	THR
2	C	569	VAL
2	C	573	ARG
2	C	578	VAL
2	C	583	LEU
2	C	584	GLU
2	C	592	LEU
2	C	599	GLU
2	C	610	ARG
2	C	613	VAL
2	C	614	ARG
2	C	620	LEU

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Mol	Chain	Res	Type
2	C	621	VAL
2	C	625	LEU
2	C	627	ARG
2	C	631	SER
2	C	632	ASN
2	C	633	GLN
2	C	635	THR
2	C	639	GLN
2	C	643	VAL
2	C	647	GLN
2	C	651	LYS
2	C	655	LEU
2	C	670	GLN
2	C	679	PHE
2	C	688	ILE
2	C	690	ILE
2	C	696	LYS
2	C	697	ARG
2	C	698	ASP
2	C	699	PHE
2	C	713	ARG
2	C	722	ILE
2	C	724	ARG
2	C	728	HIS
2	C	731	GLU
2	C	734	LEU
2	C	735	ARG
2	C	743	VAL
2	C	754	ILE
2	C	758	ARG
2	C	764	GLU
2	C	765	GLN
2	C	770	GLU
2	C	772	ARG
2	C	783	ARG
2	C	784	ASP
2	C	785	VAL
2	C	788	THR
2	C	796	GLU
2	C	799	ILE
2	C	801	VAL
2	C	803	ARG

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Mol	Chain	Res	Type
2	C	810	ASP
2	C	815	LEU
2	C	816	LYS
2	C	820	ARG
2	C	821	GLU
2	C	838	LYS
2	C	839	LEU
2	C	841	ASN
2	C	851	LYS
2	C	852	ILE
2	C	853	LEU
2	C	855	VAL
2	C	861	LEU
2	C	869	VAL
2	C	874	LEU
2	C	879	ARG
2	C	881	ASN
2	C	890	LEU
2	C	902	ILE
2	C	903	SER
2	C	905	VAL
2	C	913	GLU
2	C	915	LYS
2	C	916	GLU
2	C	918	LEU
2	C	923	ASN
2	C	924	LEU
2	C	925	TYR
2	C	930	GLN
2	C	937	ASP
2	C	938	LYS
2	C	939	ARG
2	C	950	LEU
2	C	952	LEU
2	C	960	GLU
2	C	963	LEU
2	C	966	LEU
2	C	971	LYS
2	C	972	VAL
2	C	979	THR
2	C	995	MET
2	C	1000	MET

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Mol	Chain	Res	Type
2	C	1001	VAL
2	C	1005	MET
2	C	1010	THR
2	C	1014	SER
2	C	1015	LEU
2	C	1021	LEU
2	C	1024	LYS
2	C	1027	PHE
2	C	1031	ARG
2	C	1034	GLU
2	C	1040	LEU
2	C	1050	GLN
2	C	1052	MET
2	C	1053	LEU
2	C	1055	ILE
2	C	1057	SER
2	C	1072	LYS
2	C	1078	GLU
2	C	1080	SER
2	C	1084	SER
2	C	1085	PHE
2	C	1088	LEU
2	C	1099	VAL
2	C	1100	GLN
2	C	1106	ASP
2	C	1113	GLU
3	D	5	VAL
3	D	6	ARG
3	D	9	ARG
3	D	10	ILE
3	D	12	LEU
3	D	14	SER
3	D	16	GLU
3	D	40	GLU
3	D	41	ARG
3	D	49	ILE
3	D	54	LYS
3	D	55	ASP
3	D	62	LYS
3	D	64	LYS
3	D	71	LYS
3	D	73	CYS

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Mol	Chain	Res	Type
3	D	75	ARG
3	D	81	THR
3	D	82	ARG
3	D	83	SER
3	D	84	ILE
3	D	95	LEU
3	D	97	THR
3	D	101	HIS
3	D	102	ILE
3	D	116	LEU
3	D	121	THR
3	D	122	GLU
3	D	123	LEU
3	D	128	TYR
3	D	129	PHE
3	D	134	VAL
3	D	150	ARG
3	D	154	THR
3	D	156	GLU
3	D	157	GLU
3	D	160	GLU
3	D	168	THR
3	D	176	ASP
3	D	179	VAL
3	D	183	GLU
3	D	187	LYS
3	D	189	GLN
3	D	206	ARG
3	D	209	ARG
3	D	216	LEU
3	D	219	GLU
3	D	224	ARG
3	D	225	ILE
3	D	227	LEU
3	D	237	ARG
3	D	240	GLU
3	D	241	VAL
3	D	245	LEU
3	D	250	LEU
3	D	256	SER
3	D	261	LEU
3	D	273	ARG

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Mol	Chain	Res	Type
3	D	284	LEU
3	D	289	THR
3	D	297	ILE
3	D	298	VAL
3	D	299	GLU
3	D	310	LEU
3	D	312	ARG
3	D	313	LEU
3	D	315	ARG
3	D	316	HIS
3	D	321	GLU
3	D	326	GLU
3	D	331	VAL
3	D	333	LEU
3	D	334	THR
3	D	346	LYS
3	D	354	ILE
3	D	355	VAL
3	D	357	GLU
3	D	360	LYS
3	D	371	ILE
3	D	378	ILE
3	D	388	HIS
3	D	400	VAL
3	D	406	ASP
3	D	407	VAL
3	D	411	THR
3	D	414	ARG
3	D	415	VAL
3	D	448	GLU
3	D	450	TYR
3	D	452	ILE
3	D	456	MET
3	D	459	GLU
3	D	462	GLN
3	D	464	LEU
3	D	472	LYS
3	D	473	LEU
3	D	481	MET
3	D	482	LYS
3	D	485	SER
3	D	486	ARG

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Mol	Chain	Res	Type
3	D	488	ARG
3	D	491	LYS
3	D	495	ARG
3	D	496	LEU
3	D	497	GLU
3	D	498	VAL
3	D	500	ARG
3	D	503	LEU
3	D	508	ARG
3	D	510	GLU
3	D	514	LEU
3	D	515	GLU
3	D	525	ARG
3	D	534	ARG
3	D	540	LEU
3	D	544	TYR
3	D	550	ARG
3	D	558	LEU
3	D	565	ILE
3	D	568	ARG
3	D	570	GLU
3	D	592	THR
3	D	597	GLU
3	D	600	LEU
3	D	601	ARG
3	D	603	LEU
3	D	607	LEU
3	D	610	LYS
3	D	611	GLN
3	D	613	ARG
3	D	618	LEU
3	D	619	LEU
3	D	621	LYS
3	D	622	ARG
3	D	624	ASP
3	D	626	SER
3	D	628	ARG
3	D	632	VAL
3	D	636	GLN
3	D	642	CYS
3	D	644	LEU
3	D	646	LYS

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Mol	Chain	Res	Type
3	D	647	ARG
3	D	648	MET
3	D	650	LEU
3	D	652	LEU
3	D	659	LYS
3	D	660	LYS
3	D	662	GLU
3	D	664	LYS
3	D	669	ASN
3	D	676	MET
3	D	680	GLN
3	D	682	ASP
3	D	684	LYS
3	D	691	LEU
3	D	692	GLU
3	D	700	VAL
3	D	701	LEU
3	D	709	HIS
3	D	710	ARG
3	D	711	LEU
3	D	717	GLN
3	D	720	LEU
3	D	721	VAL
3	D	747	VAL
3	D	751	LEU
3	D	752	SER
3	D	753	SER
3	D	754	PHE
3	D	760	ARG
3	D	778	LEU
3	D	780	LYS
3	D	784	ASP
3	D	787	LEU
3	D	791	TYR
3	D	792	ILE
3	D	794	GLN
3	D	797	LYS
3	D	808	THR
3	D	810	GLU
3	D	813	LEU
3	D	817	GLU
3	D	827	ILE

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Mol	Chain	Res	Type
3	D	828	VAL
3	D	832	ARG
3	D	836	VAL
3	D	838	ARG
3	D	846	PRO
3	D	857	LEU
3	D	858	LEU
3	D	860	LEU
3	D	861	GLN
3	D	866	VAL
3	D	869	LEU
3	D	871	ARG
3	D	872	ARG
3	D	875	THR
3	D	881	LEU
3	D	884	ARG
3	D	897	GLN
3	D	901	GLN
3	D	904	VAL
3	D	910	SER
3	D	913	ASP
3	D	914	LEU
3	D	917	GLN
3	D	920	LEU
3	D	921	ARG
3	D	922	LEU
3	D	930	LEU
3	D	931	LEU
3	D	932	ASP
3	D	935	LYS
3	D	936	TYR
3	D	940	THR
3	D	941	LEU
3	D	944	THR
3	D	945	SER
3	D	947	ILE
3	D	948	THR
3	D	955	VAL
3	D	960	LYS
3	D	969	ARG
3	D	974	ILE
3	D	975	GLU

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Mol	Chain	Res	Type
3	D	980	MET
3	D	984	THR
3	D	986	ARG
3	D	988	ARG
3	D	993	ILE
3	D	994	GLN
3	D	997	THR
3	D	999	THR
3	D	1009	LYS
3	D	1014	ASN
3	D	1020	LEU
3	D	1029	ARG
3	D	1034	GLN
3	D	1036	ARG
3	D	1042	ARG
3	D	1044	LEU
3	D	1049	SER
3	D	1052	THR
3	D	1058	ARG
3	D	1065	LEU
3	D	1067	VAL
3	D	1073	SER
3	D	1078	ARG
3	D	1083	ASP
3	D	1101	VAL
3	D	1104	GLU
3	D	1105	ILE
3	D	1109	GLU
3	D	1114	THR
3	D	1115	THR
3	D	1127	GLU
3	D	1129	THR
3	D	1134	LEU
3	D	1137	ARG
3	D	1141	GLU
3	D	1142	SER
3	D	1151	ARG
3	D	1158	ARG
3	D	1173	PHE
3	D	1184	ARG
3	D	1189	ARG
3	D	1190	SER

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Mol	Chain	Res	Type
3	D	1196	THR
3	D	1202	GLN
3	D	1207	TYR
3	D	1209	LEU
3	D	1213	ARG
3	D	1215	VAL
3	D	1231	GLU
3	D	1237	THR
3	D	1238	MET
3	J	1253	THR
3	J	1258	ARG
3	J	1260	ILE
3	J	1262	LEU
3	J	1269	LYS
3	J	1275	SER
3	J	1277	ILE
3	J	1281	VAL
3	J	1284	GLU
3	J	1295	GLU
3	J	1299	PHE
3	J	1302	GLU
3	J	1304	LYS
3	J	1305	LEU
3	J	1307	LYS
3	J	1311	LEU
3	J	1312	LEU
3	J	1314	LYS
3	J	1319	VAL
3	J	1320	GLU
3	J	1325	LEU
3	J	1326	THR
3	J	1327	ARG
3	J	1337	GLU
3	J	1346	ARG
3	J	1348	LEU
3	J	1355	VAL
3	J	1357	ARG
3	J	1359	GLN
3	J	1366	LYS
3	J	1370	ILE
3	J	1373	ARG
3	J	1379	VAL

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Mol	Chain	Res	Type
3	J	1382	THR
3	J	1389	LEU
3	J	1395	LEU
3	J	1397	LYS
3	J	1399	ASP
3	J	1403	LEU
3	J	1404	ASN
3	J	1412	LYS
3	J	1417	TRP
3	J	1418	LYS
3	J	1421	LEU
3	J	1422	MET
3	J	1430	SER
3	J	1432	LYS
3	J	1433	SER
3	J	1434	TRP
3	J	1435	LEU
3	J	1439	SER
3	J	1443	THR
3	J	1448	THR
3	J	1455	LYS
3	J	1458	GLU
3	J	1459	LEU
3	J	1463	LYS
3	J	1470	ARG
3	J	1472	ILE
3	J	1476	THR
3	J	1481	VAL
3	J	1482	ARG
3	J	1488	ASP
3	J	1493	LYS
3	J	1495	ILE
3	J	1496	GLU
3	J	1497	GLU
3	J	1500	LYS
4	K	6	ILE
4	K	8	LYS
4	K	16	LYS
4	K	28	GLN
4	K	29	GLN
4	K	31	LEU
4	K	36	LYS

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Mol	Chain	Res	Type
4	K	39	VAL
4	K	40	LEU
4	K	43	GLU
4	K	45	ARG
4	K	48	MET
4	K	49	ARG
4	K	50	THR
4	K	59	ASN
4	K	61	VAL
4	K	66	LYS
4	K	67	GLU
4	K	69	LEU
4	K	77	GLU
4	K	79	LEU
4	K	93	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	19	HIS
1	B	81	ASN
1	B	212	ASN
1	B	213	GLN
1	B	221	HIS
1	B	223	ASN
2	C	31	GLN
2	C	80	GLN
2	C	139	GLN
2	C	141	HIS
2	C	327	HIS
2	C	343	GLN
2	C	374	ASN
2	C	393	GLN
2	C	399	ASN
2	C	431	HIS
2	C	575	GLN
2	C	623	HIS
2	C	632	ASN
2	C	633	GLN
2	C	647	GLN
2	C	671	ASN
2	C	841	ASN

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Mol	Chain	Res	Type
2	C	860	HIS
2	C	881	ASN
2	C	889	HIS
2	C	1018	GLN
2	C	1019	GLN
2	C	1030	GLN
3	D	33	ASN
3	D	101	HIS
3	D	189	GLN
3	D	616	GLN
3	D	636	GLN
3	D	641	GLN
3	D	680	GLN
3	D	727	GLN
3	D	756	GLN
3	D	762	GLN
3	D	767	HIS
3	D	855	HIS
3	D	897	GLN
3	D	1037	GLN
3	D	1103	HIS
3	D	1202	GLN
3	J	1333	HIS
3	J	1359	GLN
3	J	1374	GLN
3	J	1465	ASN
4	K	29	GLN
4	K	59	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
5	SRN	C	1120	-	60,62,62	1.34	4 (6%)	62,84,84	1.63	10 (16%)

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
5	SRN	C	1120	-	-	10/52/105/105	0/4/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1120	SRN	O1-C1	6.91	1.48	1.34
5	C	1120	SRN	C2-C1	-4.71	1.37	1.48
5	C	1120	SRN	C5-C6	-3.50	1.34	1.44
5	C	1120	SRN	C3-C4	-3.12	1.35	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1120	SRN	O1-C1-C2	5.25	123.29	111.38
5	C	1120	SRN	O1-C33-C47	-3.80	100.97	108.85
5	C	1120	SRN	C34-C9-C10	-3.53	106.16	114.05
5	C	1120	SRN	C35-O8-C12	3.22	118.53	112.81
5	C	1120	SRN	C8-C7-C6	-3.18	119.38	125.61
5	C	1120	SRN	O1-C1-O2	-3.16	118.20	123.35
5	C	1120	SRN	C39-C38-C36	-2.66	117.85	127.09
5	C	1120	SRN	C32-C33-C47	2.53	113.21	110.64
5	C	1120	SRN	C23-C24-C25	-2.28	119.70	124.79
5	C	1120	SRN	O7-C31-C46	2.25	116.35	110.91

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1120	SRN	O7-C32-C36-C37
5	C	1120	SRN	O2-C1-O1-C33
5	C	1120	SRN	C42-C43-C44-C45
5	C	1120	SRN	C2-C1-O1-C33
5	C	1120	SRN	C39-C41-C42-C43
5	C	1120	SRN	C6-C7-C8-O3
5	C	1120	SRN	O5-C22-C23-O6
5	C	1120	SRN	O7-C32-C36-C38
5	C	1120	SRN	C14-C15-C16-O9
5	C	1120	SRN	C14-C15-C16-C17

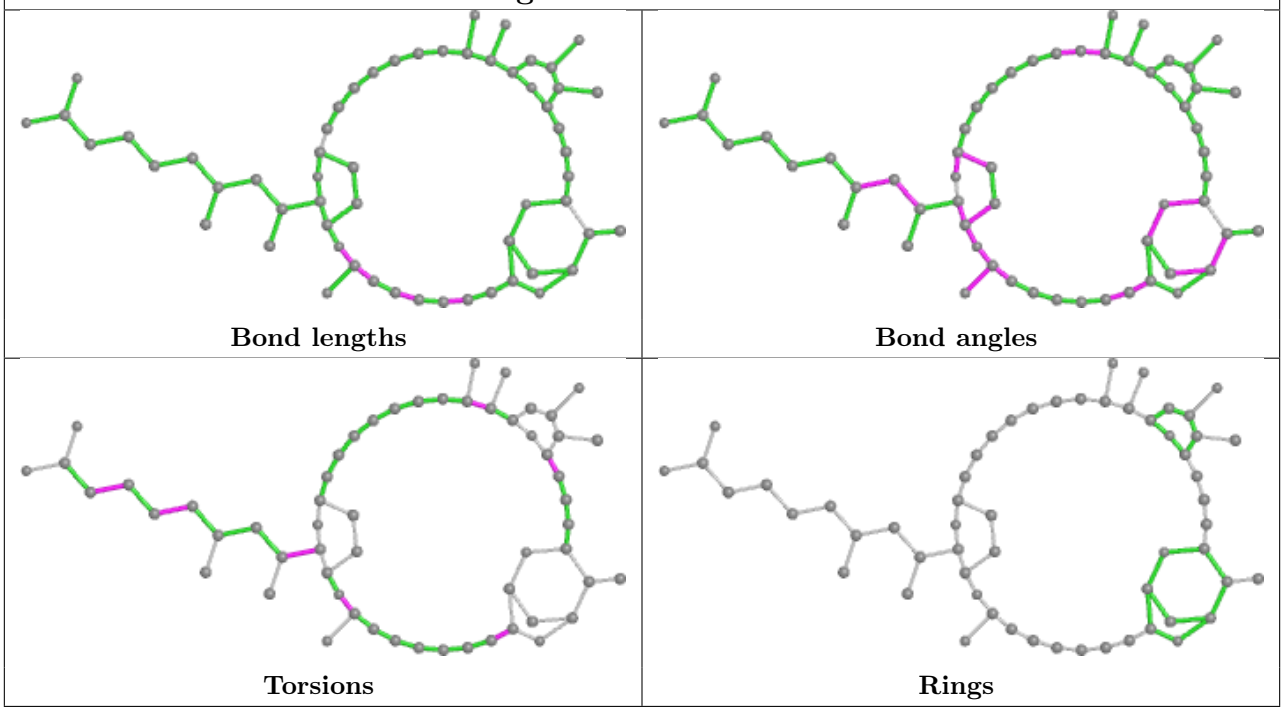
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1120	SRN	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 SRN C 1120



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	230/314 (73%)	-0.27	2 (0%)	84	75	22, 43, 76, 112	0
1	B	225/314 (71%)	-0.33	1 (0%)	92	89	24, 51, 81, 86	0
2	C	1114/1119 (99%)	-0.28	13 (1%)	79	67	19, 50, 90, 115	0
3	D	1238/1524 (81%)	-0.10	59 (4%)	30	18	18, 49, 94, 139	0
3	J	249/1524 (16%)	0.02	15 (6%)	21	12	24, 51, 125, 139	0
4	K	95/99 (95%)	-0.24	2 (2%)	63	49	27, 64, 149, 162	0
All	All	3151/4894 (64%)	-0.19	92 (2%)	51	36	18, 50, 95, 162	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	191	LEU	8.9
3	D	193	PRO	7.3
3	D	346	LYS	5.3
3	D	1240	THR	5.3
3	D	373	PRO	5.0
3	D	350	HIS	4.4
3	D	69	GLU	4.3
3	D	70	GLY	4.2
3	J	1306	PRO	4.1
3	J	1381	VAL	4.1
3	D	137	PRO	4.0
3	D	67	ARG	4.0
3	D	211	VAL	3.8
3	D	481	MET	3.8
3	J	1403	LEU	3.8
3	D	485	SER	3.8
3	D	194	GLY	3.6
3	J	1311	LEU	3.5
3	J	1287	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
3	D	831	GLY	3.5
3	D	982	PHE	3.4
3	D	1238	MET	3.3
3	D	201	GLY	3.2
3	J	1407	LEU	3.2
3	J	1498	ALA	3.2
3	D	63	TYR	3.2
3	D	336	PHE	3.2
3	D	348	ALA	3.2
3	J	1286	GLY	3.1
3	D	351	MET	3.1
3	D	68	PHE	3.0
3	D	375	GLU	3.0
3	D	370	ALA	3.0
2	C	649	VAL	3.0
1	A	234	PRO	3.0
3	D	136	ASP	2.8
3	J	1487	VAL	2.8
3	J	1308	ASP	2.7
3	D	483	HIS	2.7
3	D	532	GLY	2.7
3	D	349	PRO	2.7
3	D	208	PRO	2.6
3	J	1499	ARG	2.6
2	C	61	LYS	2.6
3	D	66	GLN	2.6
2	C	223	ASP	2.6
2	C	55	GLU	2.5
3	D	79	GLU	2.5
3	D	57	GLU	2.5
2	C	615	TYR	2.5
3	J	1290	LEU	2.5
3	J	1501	GLU	2.5
3	D	192	ALA	2.4
3	D	832	ARG	2.4
3	D	185	VAL	2.4
1	B	227	ASN	2.4
3	D	213	VAL	2.4
3	D	377	VAL	2.4
3	D	376	GLU	2.4
3	D	811	GLU	2.4
3	D	190	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	762	LYS	2.3
3	D	479	GLU	2.3
3	D	371	ILE	2.3
3	D	366	LYS	2.3
2	C	62	GLY	2.2
3	D	372	ASP	2.2
3	D	1158	ARG	2.2
4	K	92	LEU	2.2
2	C	52	PHE	2.2
3	D	81	THR	2.2
3	D	681	ARG	2.2
3	D	533	GLY	2.2
3	D	1086	LEU	2.2
2	C	213	ALA	2.2
3	D	1239	ARG	2.2
3	D	347	VAL	2.2
2	C	58	ASP	2.1
1	A	6	LEU	2.1
3	D	189	GLN	2.1
3	D	345	TYR	2.1
4	K	93	TYR	2.1
3	D	383	GLY	2.1
3	J	1313	VAL	2.1
2	C	779	GLY	2.1
3	D	209	ARG	2.1
2	C	248	PRO	2.1
3	D	367	ILE	2.1
3	D	491	LYS	2.0
3	D	80	VAL	2.0
2	C	425	PHE	2.0
3	J	1393	GLN	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

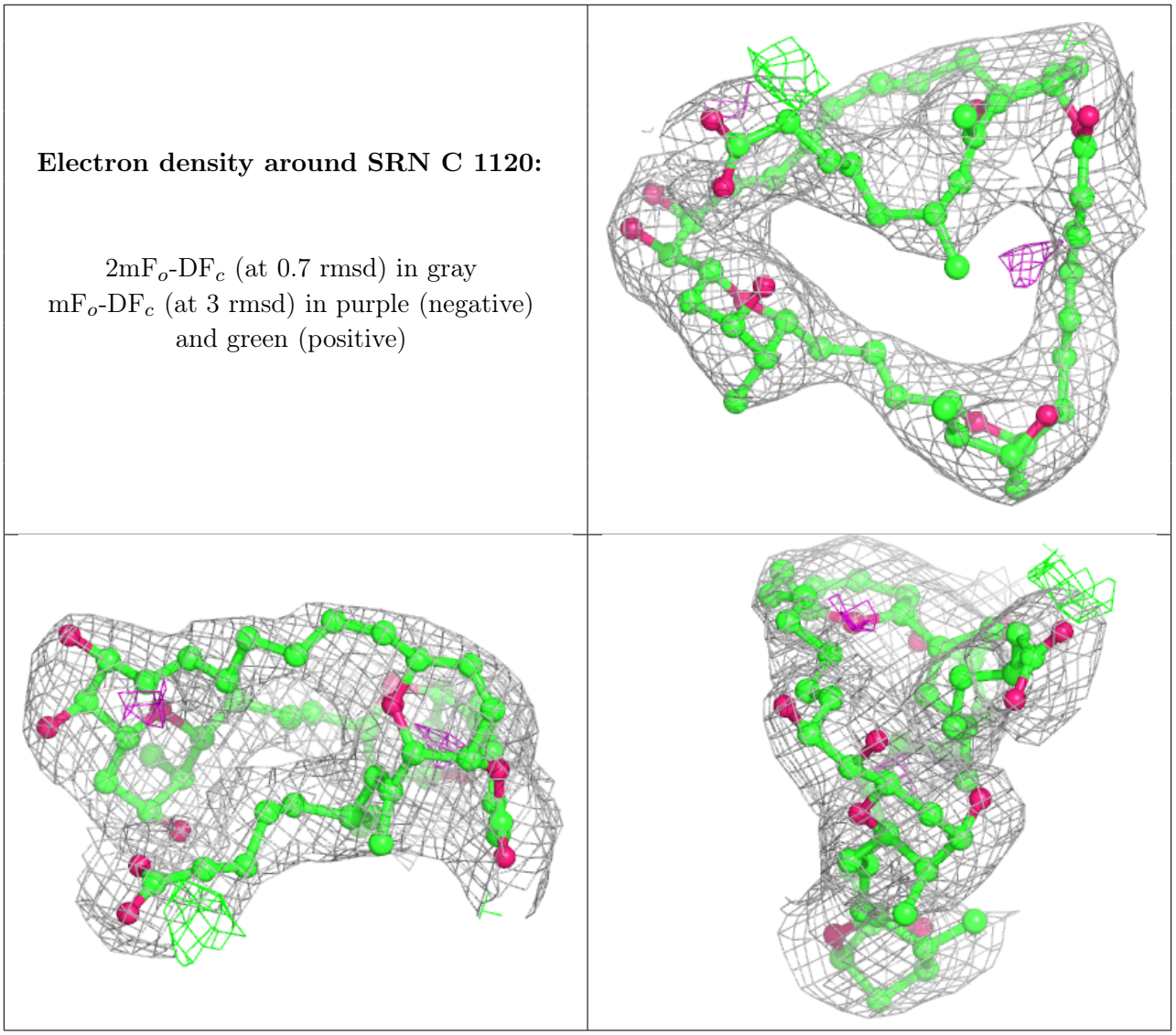
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	SRN	C	1120	58/58	0.92	0.27	33,45,56,59	0
6	ZN	D	1526	1/1	0.93	0.13	64,64,64,64	0
6	ZN	D	1525	1/1	0.96	0.03	77,77,77,77	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 SRN C 1120:

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



6.5 Other polymers (i)

There are no such residues in this entry.