



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:30 am BST

PDB ID : 1YNN
Title : Taq RNA polymerase-rifampicin 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 : 3.30 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 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 : 2.11
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) : 2.11

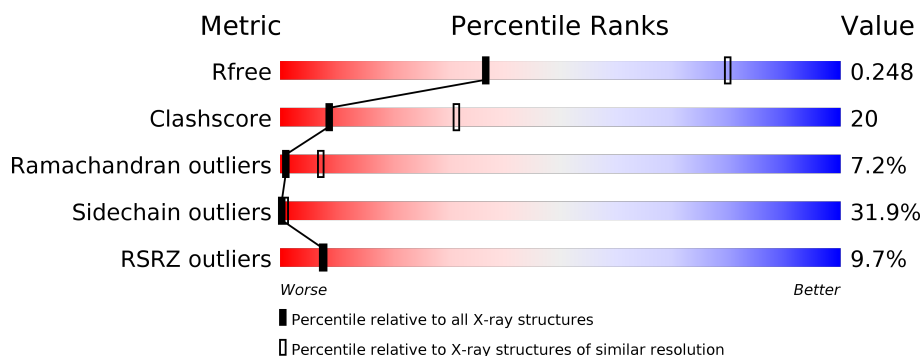
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	314	<div> <div>4%</div> <div> <div>36%</div> <div>25%</div> <div>10%</div> <div>•</div> <div>27%</div> </div> </div>
1	B	314	<div> <div>5%</div> <div> <div>31%</div> <div>29%</div> <div>10%</div> <div>•</div> <div>28%</div> </div> </div>
2	C	1119	<div> <div>5%</div> <div> <div>43%</div> <div>40%</div> <div>15%</div> <div>•</div> </div> </div>
3	D	1524	<div> <div>12%</div> <div> <div>37%</div> <div>32%</div> <div>11%</div> <div>•</div> <div>19%</div> </div> </div>
3	J	1524	<div> <div>•</div> <div> <div>8%</div> <div>5%</div> <div>•</div> <div>84%</div> </div> </div>
4	K	99	<div> <div>15%</div> <div> <div>55%</div> <div>26%</div> <div>14%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 24368 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
			8576	5430	1513	1609	24			

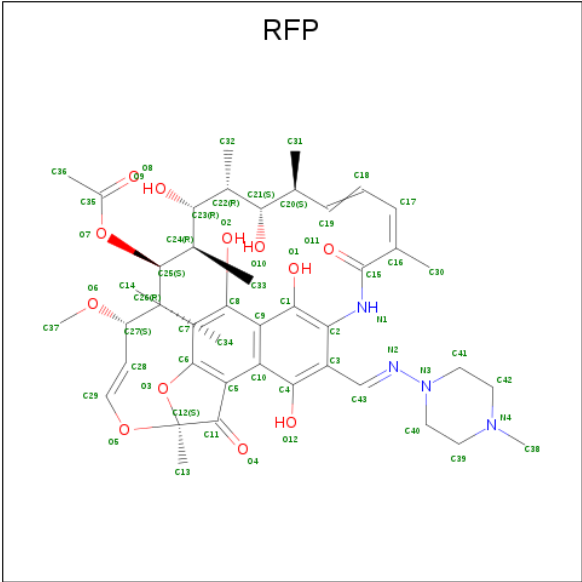
- Molecule 3 is a protein called DNA-directed RNA polymerase beta' chain.

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 RIFAMPICIN (three-letter code: RFP) (formula: C₄₃H₅₈N₄O₁₂).

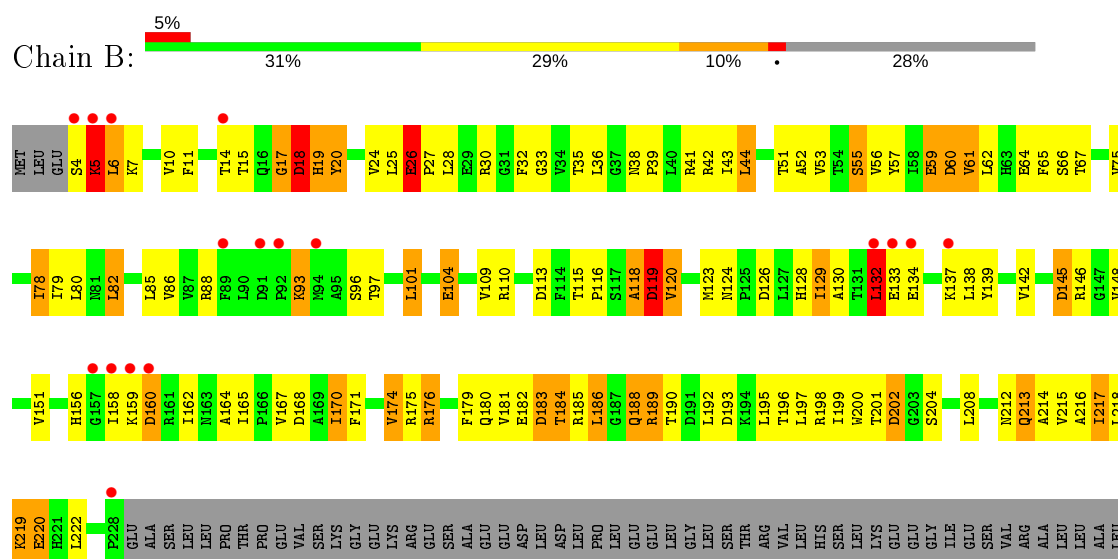


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			59	43	4	12		

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

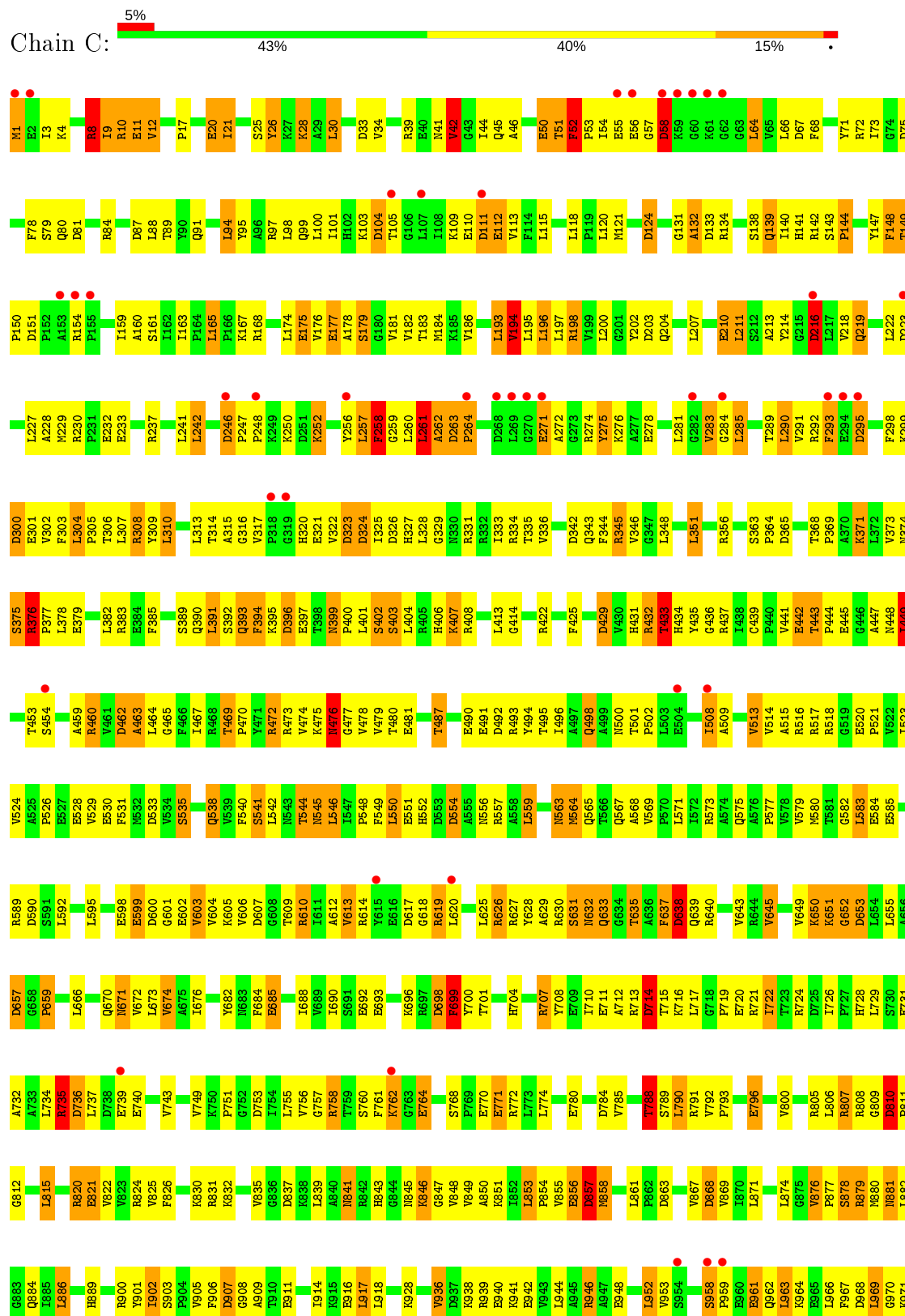
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Zn	0	0
			2	2		

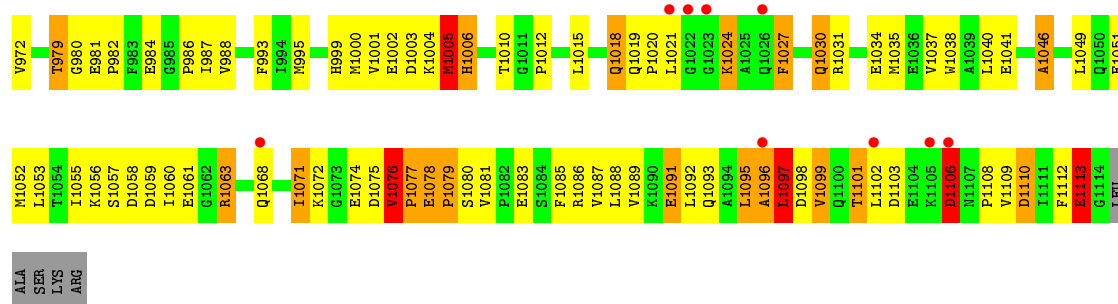
- Molecule 1: DNA-directed RNA polymerase alpha chain



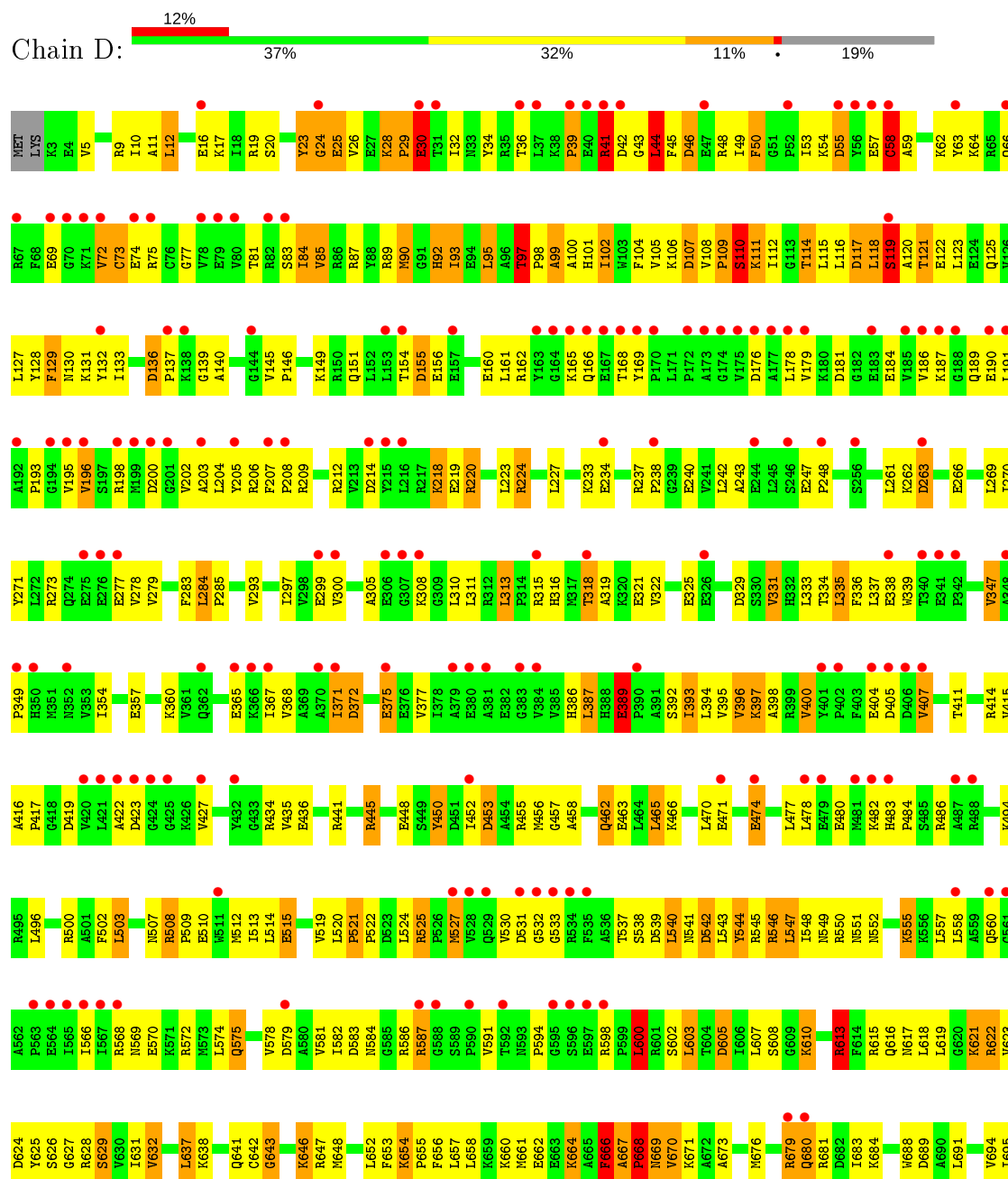
ASN LEU LYS ASP ARG ASN ILE PRO GLY ILE GLY GIU ARG SER LEU GIU GIU TLE ARG ALA ALA LYS LYS GLY PHE THR LEU LYS GIU

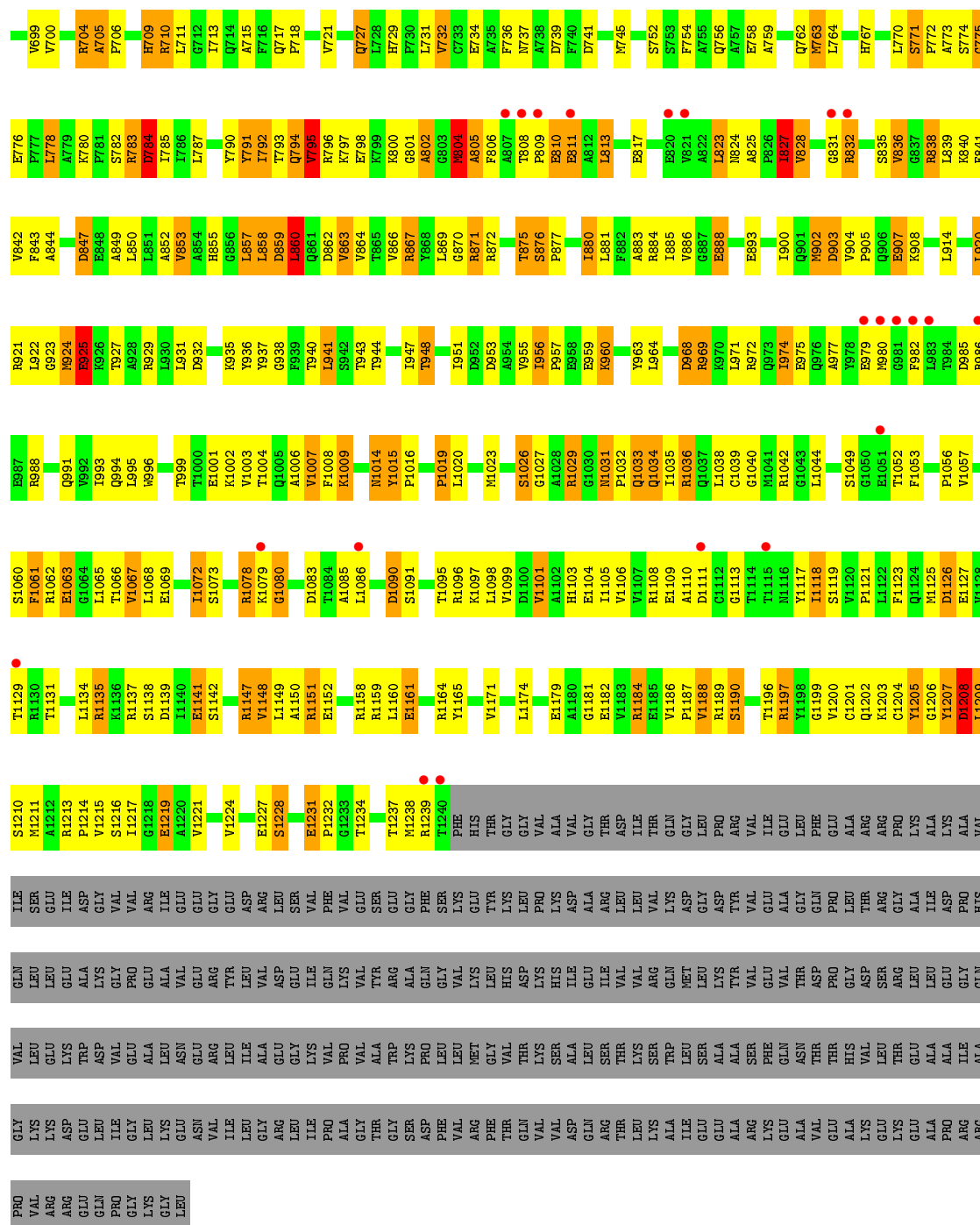
• Molecule 2: DNA-directed RNA polymerase beta chain



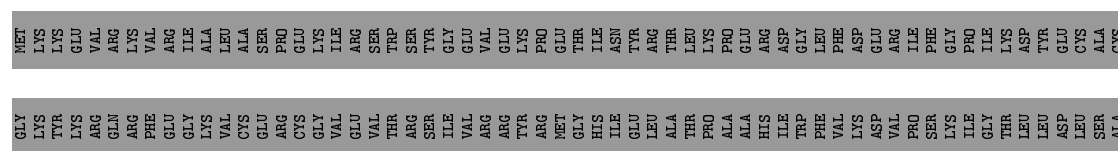


• Molecule 3: DNA-directed RNA polymerase beta' chain

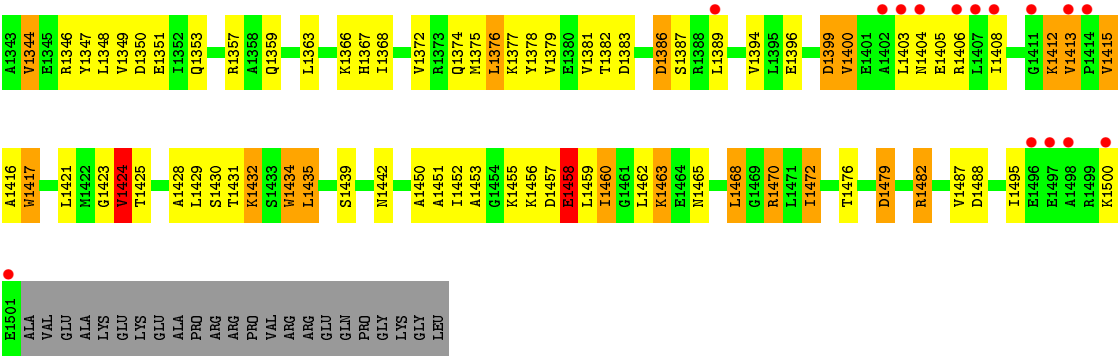




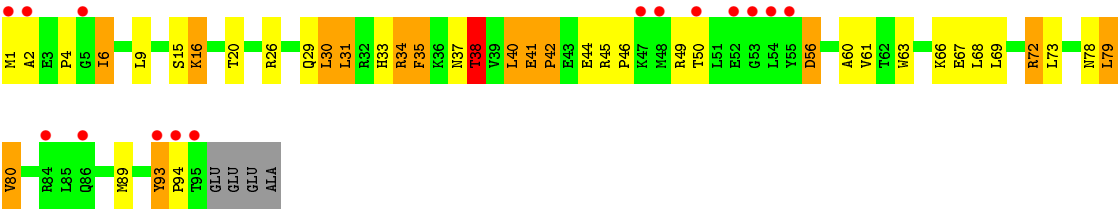
- Molecule 3: DNA-directed RNA polymerase beta' chain







● Molecule 4: DNA-directed RNA polymerase omega chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	200.76 Å 200.76 Å 292.94 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.19 – 3.23	Depositor EDS
% Data completeness (in resolution range)	84.9 (30.00-3.30) 83.4 (30.19-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.24 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.271 , 0.331 0.261 , 0.248	Depositor DCC
R_{free} test set	4075 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	87.9	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 88.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	24368	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.43	0/1798	0.84	11/2453 (0.4%)
1	B	0.41	0/1784	0.81	10/2428 (0.4%)
2	C	0.44	0/8742	0.82	41/11848 (0.3%)
3	D	0.43	0/9772	0.77	24/13234 (0.2%)
3	J	0.43	0/1897	0.75	6/2570 (0.2%)
4	K	0.45	0/762	0.74	1/1029 (0.1%)
All	All	0.43	0/24755	0.79	93/33562 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	75	ASP	CB-CG-OD2	7.29	124.86	118.30
2	C	1103	ASP	CB-CG-OD2	6.74	124.37	118.30
2	C	863	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	202	ASP	CB-CG-OD2	6.27	123.94	118.30
2	C	492	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	113	ASP	CB-CG-OD2	6.22	123.90	118.30
3	D	953	ASP	CB-CG-OD2	6.14	123.82	118.30
2	C	554	ASP	CB-CG-OD2	6.08	123.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	300	ASP	CB-CG-OD2	6.04	123.74	118.30
2	C	638	ASP	CB-CG-OD2	6.00	123.69	118.30
1	A	191	ASP	CB-CG-OD2	5.96	123.66	118.30
1	B	202	ASP	CB-CG-OD2	5.94	123.64	118.30
2	C	429	ASP	CB-CG-OD2	5.93	123.64	118.30
2	C	590	ASP	CB-CG-OD2	5.92	123.62	118.30
3	D	1139	ASP	CB-CG-OD2	5.90	123.61	118.30
2	C	133	ASP	CB-CG-OD2	5.86	123.57	118.30
3	D	539	ASP	CB-CG-OD2	5.85	123.56	118.30
3	D	739	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	132	LEU	CA-CB-CG	5.83	128.70	115.30
2	C	952	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	90	LEU	CA-CB-CG	5.82	128.68	115.30
2	C	365	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	168	ASP	CB-CG-OD2	5.79	123.51	118.30
2	C	246	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	113	ASP	CB-CG-OD2	5.77	123.49	118.30
3	D	862	ASP	CB-CG-OD2	5.73	123.46	118.30
3	D	1090	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	119	ASP	CB-CG-OD2	5.65	123.39	118.30
2	C	868	ASP	CB-CG-OD2	5.65	123.38	118.30
2	C	969	LEU	CA-CB-CG	5.63	128.26	115.30
2	C	216	ASP	CB-CG-OD2	5.63	123.37	118.30
3	D	784	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	60	ASP	CB-CG-OD2	5.59	123.33	118.30
2	C	837	ASP	CB-CG-OD2	5.58	123.33	118.30
2	C	67	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	145	ASP	CB-CG-OD2	5.57	123.31	118.30
3	D	107	ASP	CB-CG-OD2	5.54	123.29	118.30
2	C	104	ASP	CB-CG-OD2	5.51	123.26	118.30
3	D	453	ASP	CB-CG-OD2	5.50	123.25	118.30
3	J	1479	ASP	CB-CG-OD2	5.49	123.24	118.30
2	C	52	PHE	N-CA-C	5.49	125.82	111.00
2	C	81	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	18	ASP	CB-CG-OD2	5.48	123.23	118.30
3	D	423	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	145	ASP	CB-CG-OD2	5.47	123.22	118.30
3	J	1317	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	74	ASP	CB-CG-OD2	5.46	123.22	118.30
2	C	653	ASP	CB-CG-OD2	5.45	123.21	118.30
2	C	559	LEU	CA-CB-CG	5.45	127.83	115.30
2	C	342	ASP	CB-CG-OD2	5.42	123.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1208	ASP	CB-CG-OD2	5.41	123.16	118.30
2	C	58	ASP	CB-CG-OD2	5.40	123.16	118.30
3	J	1386	ASP	CB-CG-OD2	5.39	123.15	118.30
3	D	372	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	160	ASP	CB-CG-OD2	5.38	123.14	118.30
3	D	263	ASP	CB-CG-OD2	5.38	123.14	118.30
3	J	1315	ASP	CB-CG-OD2	5.36	123.12	118.30
4	K	56	ASP	CB-CG-OD2	5.36	123.12	118.30
2	C	857	ASP	CB-CG-OD2	5.35	123.11	118.30
3	J	1488	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	60	ASP	CB-CG-OD2	5.33	123.10	118.30
3	D	1126	ASP	CB-CG-OD2	5.33	123.09	118.30
2	C	1003	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	193	ASP	CB-CG-OD2	5.32	123.08	118.30
3	D	847	ASP	CB-CG-OD2	5.30	123.07	118.30
2	C	203	ASP	CB-CG-OD2	5.29	123.06	118.30
3	D	605	ASP	CB-CG-OD2	5.29	123.06	118.30
3	D	903	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	168	ASP	CB-CG-OD2	5.28	123.05	118.30
2	C	396	ASP	CB-CG-OD2	5.27	123.05	118.30
2	C	324	ASP	CB-CG-OD2	5.26	123.04	118.30
3	D	200	ASP	CB-CG-OD2	5.26	123.03	118.30
2	C	839	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	183	ASP	CB-CG-OD2	5.22	123.00	118.30
3	D	55	ASP	CB-CG-OD2	5.20	122.98	118.30
2	C	736	ASP	CB-CG-OD2	5.20	122.98	118.30
3	D	117	ASP	CB-CG-OD2	5.19	122.97	118.30
3	J	1350	ASP	CB-CG-OD2	5.18	122.96	118.30
2	C	657	ASP	CB-CG-OD2	5.18	122.96	118.30
2	C	810	ASP	CB-CG-OD2	5.17	122.96	118.30
2	C	151	ASP	CB-CG-OD2	5.16	122.94	118.30
2	C	698	ASP	CB-CG-OD2	5.16	122.94	118.30
3	D	155	ASP	CB-CG-OD2	5.15	122.93	118.30
3	D	542	ASP	CB-CG-OD2	5.14	122.93	118.30
3	D	985	ASP	CB-CG-OD2	5.12	122.91	118.30
2	C	1106	ASP	CB-CG-OD2	5.11	122.90	118.30
2	C	1110	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	18	ASP	CB-CG-OD2	5.09	122.88	118.30
2	C	714	ASP	CB-CG-OD2	5.08	122.88	118.30
1	B	160	ASP	CB-CG-OD2	5.08	122.88	118.30
3	D	181	ASP	CB-CG-OD2	5.06	122.85	118.30
2	C	295	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	223	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	125	PRO	Peptide
2	C	51	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1760	65	0
1	B	1750	0	1775	69	0
2	C	8576	0	8510	406	0
3	D	9602	0	9558	427	0
3	J	1869	0	1876	75	0
4	K	747	0	735	22	0
5	C	59	0	55	10	0
6	D	2	0	0	0	0
All	All	24368	0	24269	995	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 20.

All (995) 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:136:ASP:HB3	3:D:137:PRO:HD3	1.14	1.10
2:C:432:ARG:O	2:C:433:THR:HB	1.49	1.09
2:C:263:ASP:HB3	2:C:264:PRO:HD3	1.12	1.09
1:B:26:GLU:HB3	1:B:27:PRO:HD3	1.29	1.09
2:C:650:LYS:HB3	2:C:653:ASP:HB2	1.35	1.07
3:D:28:LYS:HG3	3:D:42:ASP:HB3	1.10	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:705:ALA:HB1	3:D:706:PRO:CD	1.85	1.05
3:D:136:ASP:HB3	3:D:137:PRO:CD	1.87	1.04
2:C:442:GLU:O	2:C:442:GLU:HG3	1.55	1.02
3:D:1101:VAL:HG21	3:J:1424:VAL:HG22	1.41	1.02
3:J:1460:ILE:HD12	3:J:1460:ILE:H	1.23	1.02
3:D:705:ALA:CB	3:D:706:PRO:HD2	1.90	1.01
3:D:136:ASP:CB	3:D:137:PRO:HD3	1.90	1.01
3:D:30:GLU:HG3	3:D:545:ARG:HD2	1.41	1.00
3:D:805:ALA:HB3	3:D:832:ARG:H	1.20	1.00
2:C:474:VAL:HG21	2:C:529:VAL:CG1	1.92	1.00
2:C:1076:VAL:HB	2:C:1077:PRO:HD3	1.43	0.98
3:D:705:ALA:HB1	3:D:706:PRO:HD2	0.98	0.98
1:B:26:GLU:CB	1:B:27:PRO:HD3	1.94	0.97
3:D:98:PRO:HB2	3:D:458:ALA:HB3	1.46	0.97
2:C:650:LYS:CB	2:C:653:ASP:HB2	1.96	0.95
2:C:211:LEU:HD11	2:C:308:ARG:HA	1.49	0.94
2:C:263:ASP:CB	2:C:264:PRO:HD3	1.98	0.94
3:D:957:PRO:HD3	3:D:1007:VAL:HG23	1.45	0.94
3:D:655:PRO:HA	3:D:658:LEU:HD12	1.47	0.94
1:B:26:GLU:HB3	1:B:27:PRO:CD	1.98	0.93
3:D:28:LYS:HG3	3:D:42:ASP:CB	1.98	0.93
4:K:41:GLU:HG3	4:K:45:ARG:HH21	1.34	0.93
3:D:1161:GLU:HG3	3:D:1164:ARG:HG3	1.50	0.91
3:D:98:PRO:CB	3:D:458:ALA:HB3	2.01	0.91
3:D:783:ARG:HG3	3:D:783:ARG:HH11	1.37	0.90
3:D:806:PHE:HB2	3:D:808:THR:O	1.70	0.90
2:C:396:ASP:H	2:C:406:HIS:HD2	1.19	0.90
2:C:601:GLY:H	2:C:649:VAL:HG22	1.37	0.90
2:C:263:ASP:HB3	2:C:264:PRO:CD	2.01	0.89
3:D:699:VAL:H	3:D:756:GLN:NE2	1.72	0.88
3:D:841:PHE:HB2	3:D:864:VAL:HG13	1.54	0.88
3:D:28:LYS:CG	3:D:42:ASP:HB3	2.03	0.88
3:D:792:ILE:HD11	3:D:881:LEU:HD23	1.56	0.88
3:D:643:GLY:HA3	3:D:727:GLN:H	1.39	0.87
3:D:870:GLY:O	3:D:871:ARG:HB2	1.74	0.86
2:C:1076:VAL:CB	2:C:1077:PRO:HD3	2.05	0.85
3:J:1275:SER:OG	3:J:1294:VAL:HG21	1.77	0.85
2:C:474:VAL:HG21	2:C:529:VAL:HG13	1.58	0.85
3:D:1147:ARG:HB3	3:D:1188:VAL:HG21	1.57	0.84
2:C:577:PRO:HA	2:C:671:ASN:ND2	1.92	0.84
2:C:628:TYR:H	2:C:638:ASP:HB2	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:563:ASN:O	2:C:565:GLN:N	2.11	0.83
3:D:859:ASP:O	3:D:860:LEU:HB2	1.77	0.83
3:D:805:ALA:HB3	3:D:832:ARG:N	1.93	0.83
3:D:828:VAL:HG11	3:D:863:VAL:H	1.43	0.83
1:A:202:ASP:O	1:A:204:SER:N	2.12	0.82
1:A:126:ASP:O	1:A:127:LEU:HB3	1.79	0.82
2:C:874:LEU:O	3:D:1029:ARG:HD2	1.79	0.82
3:D:1148:VAL:HG21	3:D:1203:LYS:O	1.80	0.82
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	1.62	0.82
3:D:1207:TYR:HA	3:D:1213:ARG:O	1.79	0.81
2:C:508:ILE:HD13	2:C:526:PRO:HB3	1.62	0.81
2:C:749:VAL:CG1	2:C:792:VAL:HG21	2.12	0.80
2:C:722:ILE:HG22	2:C:722:ILE:O	1.79	0.80
3:D:1068:LEU:O	3:D:1072:ILE:HG12	1.82	0.80
1:B:44:LEU:O	1:B:174:VAL:HG21	1.82	0.80
3:J:1264:GLU:OE2	3:J:1264:GLU:HA	1.81	0.80
2:C:637:PHE:HD1	2:C:659:PRO:HG3	1.48	0.79
2:C:575:GLN:HE21	2:C:670:GLN:HB3	1.48	0.79
3:D:843:PHE:HB2	3:D:866:VAL:HG22	1.63	0.79
3:D:1197:ARG:HD2	3:J:1396:GLU:HB3	1.64	0.79
1:B:33:GLY:O	1:B:195:LEU:HD13	1.83	0.78
3:D:100:ALA:N	3:D:575:GLN:OE1	2.17	0.78
2:C:1076:VAL:HB	2:C:1077:PRO:CD	2.12	0.78
2:C:946:ARG:HD2	2:C:984:GLU:HB2	1.65	0.78
3:D:1231:GLU:HG3	3:D:1232:PRO:HD3	1.66	0.78
1:A:198:ARG:O	1:A:199:ILE:HB	1.82	0.77
3:D:543:LEU:HD11	3:D:584:ASN:HD22	1.49	0.77
3:D:477:LEU:HA	3:D:480:GLU:HB2	1.66	0.77
2:C:693:GLU:HA	2:C:696:LYS:HD2	1.65	0.77
1:A:20:TYR:HD2	1:A:21:GLY:N	1.83	0.77
1:B:39:PRO:O	1:B:43:ILE:HD12	1.85	0.77
2:C:140:ILE:HG22	2:C:333:ILE:HD13	1.65	0.77
3:D:1211:MET:HB2	3:D:1213:ARG:HD2	1.67	0.76
3:D:937:TYR:HB3	3:D:941:LEU:HD22	1.67	0.76
2:C:1112:PHE:O	2:C:1113:GLU:HB3	1.85	0.76
2:C:1087:VAL:O	2:C:1091:GLU:HG2	1.86	0.76
2:C:565:GLN:HA	2:C:995:MET:CE	2.16	0.75
3:D:1205:TYR:CE1	3:D:1221:VAL:HG11	2.22	0.75
3:D:704:ARG:HB2	3:D:745:MET:HG3	1.67	0.75
2:C:632:ASN:HB3	2:C:633:GLN:NE2	2.01	0.74
3:D:1031:ASN:HD21	3:D:1033:GLN:HG2	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1457:ASP:O	3:J:1458:GLU:HB2	1.86	0.74
1:A:59:GLU:HG2	1:A:139:TYR:HB3	1.68	0.74
3:D:795:VAL:HG12	3:D:863:VAL:HG22	1.69	0.73
1:A:225:PHE:HD2	1:B:11:PHE:CE1	2.06	0.73
2:C:565:GLN:HA	2:C:995:MET:HE3	1.69	0.73
2:C:841:ASN:C	2:C:841:ASN:HD22	1.91	0.73
3:D:841:PHE:HB2	3:D:864:VAL:CG1	2.18	0.73
1:A:124:ASN:ND2	1:A:127:LEU:HD22	2.03	0.73
2:C:261:LEU:HD21	2:C:263:ASP:HB2	1.70	0.73
3:D:552:ASN:HA	3:D:555:LYS:HB2	1.71	0.73
2:C:600:ASP:HB3	2:C:651:LYS:HG3	1.70	0.73
2:C:432:ARG:O	2:C:433:THR:CB	2.35	0.73
3:D:62:LYS:HG3	3:D:63:TYR:H	1.54	0.73
2:C:140:ILE:CG2	2:C:333:ILE:HD13	2.19	0.73
2:C:551:GLU:HA	2:C:906:PHE:HE2	1.54	0.72
2:C:719:PRO:HD2	2:C:761:PHE:CE1	2.23	0.72
2:C:936:VAL:HA	2:C:940:GLU:OE2	1.88	0.72
2:C:672:VAL:HG22	2:C:868:ASP:HB2	1.70	0.72
2:C:477:GLY:HA2	2:C:508:ILE:HD11	1.70	0.72
3:D:220:ARG:HH21	3:D:336:PHE:HB2	1.55	0.72
3:D:850:LEU:HA	3:D:853:VAL:HG23	1.70	0.72
1:B:18:ASP:CG	1:B:19:HIS:H	1.93	0.72
2:C:1077:PRO:O	2:C:1078:GLU:HB2	1.90	0.72
2:C:3:ILE:HG23	2:C:902:ILE:HD13	1.72	0.71
2:C:1041:GLU:HG2	3:J:1472:ILE:HD11	1.72	0.71
3:D:270:ILE:HD12	3:D:284:LEU:HD21	1.70	0.71
2:C:441:VAL:HG12	2:C:442:GLU:H	1.54	0.71
2:C:258:PHE:N	2:C:258:PHE:CD1	2.58	0.71
2:C:437:ARG:NH2	2:C:491:GLU:OE1	2.24	0.71
3:D:176:ASP:HA	3:D:389:GLU:HB3	1.73	0.70
3:D:805:ALA:C	3:D:832:ARG:HB2	2.11	0.70
3:D:140:ALA:H	3:D:452:ILE:HG22	1.55	0.70
2:C:1051:GLU:HG2	2:C:1055:ILE:HD11	1.74	0.69
2:C:149:THR:HG22	2:C:150:PRO:HD2	1.72	0.69
2:C:1005:MET:HB2	3:D:629:SER:HB2	1.74	0.69
3:D:787:LEU:HG	3:D:947:ILE:HD11	1.73	0.69
4:K:26:ARG:NE	4:K:67:GLU:OE2	2.26	0.69
3:D:704:ARG:NH1	3:D:737:ASN:O	2.25	0.69
2:C:808:ARG:HB2	2:C:820:ARG:HB2	1.75	0.69
3:D:963:TYR:HE2	3:D:1002:LYS:CB	2.05	0.69
3:D:843:PHE:CE1	3:D:864:VAL:HG11	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:850:ALA:HA	3:D:632:VAL:HG21	1.73	0.69
2:C:182:VAL:HG11	2:C:307:LEU:HD11	1.75	0.69
2:C:988:VAL:HG12	3:D:948:THR:OG1	1.92	0.69
3:D:1095:THR:O	3:D:1099:VAL:HG23	1.92	0.69
2:C:474:VAL:HG21	2:C:529:VAL:HG12	1.73	0.69
2:C:632:ASN:C	2:C:633:GLN:HE21	1.96	0.69
2:C:606:VAL:HB	2:C:645:VAL:HG22	1.74	0.69
5:C:1120:RFP:HN1	5:C:1120:RFP:H18C	1.57	0.68
2:C:328:LEU:HB2	2:C:433:THR:HG23	1.74	0.68
3:D:643:GLY:HA3	3:D:727:GLN:N	2.08	0.68
1:A:158:ILE:H	1:A:166:PRO:HB3	1.56	0.68
3:D:283:PHE:CD2	3:D:335:LEU:HD13	2.29	0.68
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.23	0.68
3:D:1147:ARG:HB3	3:D:1188:VAL:CG2	2.22	0.68
2:C:134:ARG:HA	2:C:394:PHE:O	1.93	0.68
3:D:12:LEU:HB2	3:D:507:ASN:ND2	2.09	0.68
2:C:1059:ASP:OD2	2:C:1083:GLU:HB2	1.94	0.68
3:D:699:VAL:H	3:D:756:GLN:HE22	1.42	0.68
2:C:682:TYR:CE1	2:C:851:LYS:HE3	2.28	0.67
2:C:751:PRO:HA	2:C:792:VAL:HG12	1.75	0.67
3:D:1197:ARG:CD	3:J:1396:GLU:HB3	2.24	0.67
2:C:289:THR:HG22	2:C:303:PHE:CE1	2.29	0.67
2:C:17:PRO:HD2	2:C:20:GLU:HG3	1.75	0.67
3:D:783:ARG:O	3:D:784:ASP:HB2	1.94	0.67
2:C:535:SER:O	2:C:538:GLN:HB2	1.94	0.67
2:C:722:ILE:CG2	2:C:722:ILE:O	2.43	0.67
3:D:1204:CYS:O	3:D:1206:GLY:N	2.28	0.67
2:C:757:GLY:HA2	2:C:789:SER:OG	1.94	0.67
3:D:1040:GLY:O	3:D:1060:SER:HB3	1.95	0.67
2:C:551:GLU:HA	2:C:906:PHE:CE2	2.29	0.67
3:J:1372:VAL:HA	3:J:1375:MET:HE2	1.77	0.66
1:B:17:GLY:O	1:B:18:ASP:HB3	1.95	0.66
2:C:1101:THR:HB	2:C:1109:VAL:HG12	1.78	0.66
2:C:374:ASN:HB3	2:C:377:PRO:HD2	1.77	0.66
2:C:710:ILE:HB	2:C:790:LEU:HD22	1.77	0.66
2:C:1087:VAL:O	2:C:1091:GLU:CG	2.43	0.66
2:C:198:ARG:HD3	2:C:228:ALA:HA	1.77	0.66
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.36	0.66
2:C:987:ILE:HA	3:D:948:THR:HG21	1.77	0.66
2:C:701:THR:HG22	2:C:832:LYS:HA	1.78	0.66
2:C:1077:PRO:HG2	2:C:1079:PRO:HD3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:O	1:A:74:ASP:HB3	1.95	0.65
2:C:577:PRO:HA	2:C:671:ASN:HD22	1.60	0.65
3:D:1105:ILE:HD11	3:J:1374:GLN:NE2	2.11	0.65
3:D:1031:ASN:HD21	3:D:1033:GLN:CG	2.08	0.65
2:C:271:GLU:HB3	2:C:464:LEU:HD22	1.79	0.65
3:D:224:ARG:HG3	3:D:331:VAL:O	1.97	0.65
1:A:9:PRO:HA	1:A:27:PRO:HD2	1.77	0.65
3:D:1211:MET:CB	3:D:1213:ARG:HD2	2.26	0.65
3:D:715:ALA:HB3	3:D:764:LEU:HA	1.77	0.64
3:D:10:ILE:HG23	3:J:1451:ALA:HA	1.77	0.64
3:D:792:ILE:HG13	3:D:941:LEU:HG	1.79	0.64
3:D:859:ASP:O	3:D:860:LEU:CB	2.46	0.64
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.79	0.64
2:C:399:ASN:HD22	2:C:401:LEU:H	1.44	0.64
3:D:631:ILE:HG21	3:D:745:MET:SD	2.37	0.64
3:D:243:ALA:HB3	3:D:311:LEU:HD12	1.80	0.64
2:C:1056:LYS:O	3:D:624:ASP:HB2	1.98	0.64
2:C:743:VAL:HG11	2:C:800:VAL:HG21	1.78	0.64
3:D:145:VAL:CB	3:D:146:PRO:HD2	2.28	0.64
1:A:231:SER:HA	1:B:14:THR:HA	1.79	0.64
2:C:881:ASN:HD22	2:C:881:ASN:H	1.43	0.64
2:C:393:GLN:HG3	2:C:406:HIS:HE1	1.62	0.64
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.63	0.64
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.79	0.64
2:C:261:LEU:HD21	2:C:263:ASP:CB	2.27	0.63
2:C:496:ILE:O	2:C:515:ALA:HB1	1.98	0.63
1:B:57:TYR:HB2	1:B:164:ALA:HB2	1.81	0.63
3:D:1237:THR:HG22	3:D:1239:ARG:H	1.63	0.63
2:C:1076:VAL:CG1	2:C:1077:PRO:HD3	2.28	0.63
3:D:1208:ASP:C	3:D:1210:SER:H	2.01	0.63
3:D:643:GLY:CA	3:D:727:GLN:H	2.09	0.63
3:D:318:THR:HG22	3:D:338:GLU:HB2	1.81	0.63
3:D:623:VAL:HG12	3:D:625:TYR:H	1.64	0.63
2:C:469:THR:HG22	2:C:470:PRO:HD2	1.80	0.63
2:C:1098:ASP:HB3	3:D:11:ALA:HB3	1.80	0.62
2:C:601:GLY:H	2:C:649:VAL:CG2	2.10	0.62
3:D:116:LEU:HD11	3:D:465:LEU:HD23	1.81	0.62
3:J:1282:ARG:HB3	3:J:1293:PHE:HB2	1.81	0.62
2:C:672:VAL:HG22	2:C:868:ASP:CB	2.27	0.62
3:J:1396:GLU:HA	3:J:1399:ASP:HB2	1.82	0.62
2:C:575:GLN:HE21	2:C:670:GLN:CB	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:580:MET:HB3	2:C:584:GLU:CD	2.19	0.62
1:B:183:ASP:OD1	1:B:183:ASP:N	2.32	0.62
2:C:343:GLN:HG2	2:C:385:PHE:HB2	1.82	0.62
3:D:1158:ARG:HH11	3:D:1160:LEU:HD21	1.65	0.62
2:C:879:ARG:HD3	2:C:879:ARG:H	1.65	0.62
2:C:403:SER:O	2:C:407:LYS:HD2	2.00	0.62
2:C:650:LYS:C	2:C:652:GLY:H	2.01	0.62
2:C:1018:GLN:NE2	2:C:1063:ARG:HH22	1.98	0.61
2:C:707:ARG:HB2	2:C:826:PHE:CD2	2.35	0.61
3:J:1378:TYR:HE2	3:J:1394:VAL:HG22	1.64	0.61
2:C:850:ALA:HA	3:D:632:VAL:CG2	2.28	0.61
3:D:662:GLU:OE1	3:D:670:VAL:HG22	2.00	0.61
2:C:676:ILE:O	3:D:948:THR:HB	2.00	0.61
3:J:1258:ARG:CG	3:J:1258:ARG:HH11	2.13	0.61
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.82	0.61
3:D:1103:HIS:HD2	3:J:1462:LEU:H	1.48	0.61
1:A:56:VAL:HG12	1:A:142:VAL:HG12	1.82	0.61
2:C:708:TYR:OH	2:C:796:GLU:HG2	2.00	0.61
1:A:233:LEU:HB2	1:B:14:THR:HG22	1.82	0.61
2:C:72:ARG:NH1	2:C:112:GLU:OE1	2.34	0.61
4:K:46:PRO:HG2	4:K:63:TRP:NE1	2.14	0.61
2:C:944:LEU:HD11	2:C:963:LEU:HD23	1.82	0.61
2:C:674:VAL:HB	2:C:869:VAL:HG13	1.83	0.61
2:C:876:VAL:O	2:C:879:ARG:O	2.18	0.61
3:D:806:PHE:CD1	3:D:809:PRO:HA	2.36	0.61
3:D:1205:TYR:HD2	3:D:1215:VAL:HG21	1.66	0.60
3:D:642:CYS:HB3	3:D:718:PRO:HA	1.83	0.60
3:D:774:SER:O	3:D:776:GLU:N	2.34	0.60
3:D:1035:ILE:HA	3:D:1038:LEU:HD12	1.83	0.60
2:C:717:LEU:HD12	3:D:533:GLY:HA2	1.82	0.60
2:C:944:LEU:HD22	2:C:962:GLN:HB3	1.84	0.60
3:D:617:ASN:OD1	3:D:621:LYS:HE3	2.01	0.60
3:D:704:ARG:HB2	3:D:745:MET:CG	2.32	0.60
3:D:783:ARG:HG3	3:D:783:ARG:NH1	2.15	0.60
1:B:213:GLN:O	1:B:217:ILE:HG12	2.00	0.60
2:C:1081:VAL:HB	2:C:1086:ARG:NH2	2.17	0.60
2:C:682:TYR:CE1	2:C:851:LYS:CE	2.84	0.60
3:D:133:ILE:HA	3:D:456:MET:HG3	1.83	0.60
3:D:618:LEU:HD22	3:J:1463:LYS:HG3	1.83	0.60
3:D:1105:ILE:HD11	3:J:1374:GLN:HE22	1.67	0.60
3:D:1224:VAL:O	3:D:1228:SER:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:98:PRO:HB3	3:D:458:ALA:HB3	1.81	0.59
2:C:64:LEU:HD23	2:C:100:LEU:HD21	1.83	0.59
2:C:196:LEU:O	2:C:200:LEU:HG	2.02	0.59
2:C:551:GLU:HG3	2:C:906:PHE:HD2	1.66	0.59
3:D:849:ALA:O	3:D:852:ALA:HB3	2.02	0.59
1:A:149:GLY:O	1:A:171:PHE:HB2	2.03	0.59
2:C:281:LEU:HD11	2:C:306:THR:HA	1.83	0.59
2:C:399:ASN:HB2	2:C:400:PRO:HD2	1.84	0.59
3:D:416:ALA:HB1	3:D:417:PRO:CD	2.32	0.59
2:C:1019:GLN:HB2	2:C:1020:PRO:HD2	1.83	0.59
4:K:79:LEU:O	4:K:80:VAL:HB	2.02	0.59
1:A:29:GLU:O	1:A:32:PHE:HB2	2.02	0.59
2:C:626:ARG:H	2:C:639:GLN:HE21	1.49	0.59
3:D:1029:ARG:HH11	3:D:1029:ARG:HG2	1.67	0.59
3:D:1121:PRO:O	3:D:1135:ARG:HD2	2.02	0.59
3:D:97:THR:CB	3:D:98:PRO:HD3	2.32	0.59
3:J:1479:ASP:OD1	3:J:1482:ARG:NH1	2.36	0.59
1:B:185:ARG:HA	1:B:190:THR:HA	1.85	0.59
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.85	0.59
3:D:796:ARG:HH11	3:D:796:ARG:HG3	1.68	0.59
5:C:1120:RFP:H372	5:C:1120:RFP:H363	1.85	0.59
3:J:1400:VAL:O	3:J:1404:ASN:HB3	2.03	0.59
2:C:676:ILE:HB	2:C:988:VAL:HG13	1.85	0.58
1:A:133:GLU:HG2	1:A:134:GLU:N	2.17	0.58
3:D:578:VAL:O	3:D:582:ILE:HG12	2.02	0.58
2:C:1101:THR:HG22	3:D:5:VAL:HG13	1.85	0.58
5:C:1120:RFP:N1	5:C:1120:RFP:N2	2.51	0.58
3:D:218:LYS:HA	3:D:337:LEU:O	2.03	0.58
3:J:1404:ASN:C	3:J:1406:ARG:H	2.06	0.58
3:D:1078:ARG:C	3:D:1080:GLY:H	2.06	0.58
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.85	0.58
3:J:1330:ILE:O	3:J:1332:PRO:HD3	2.02	0.58
3:J:1425:THR:O	3:J:1428:ALA:HB3	2.04	0.58
1:A:225:PHE:HD2	1:B:11:PHE:HE1	1.49	0.58
1:B:18:ASP:CG	1:B:19:HIS:N	2.57	0.58
3:D:843:PHE:HE1	3:D:864:VAL:HG11	1.66	0.58
2:C:545:ASN:HB3	2:C:583:LEU:HD12	1.84	0.58
1:B:80:LEU:HB3	3:D:867:ARG:HH11	1.69	0.58
1:A:160:ASP:O	1:A:161:ARG:HB3	2.02	0.58
3:D:1006:ALA:HA	3:D:1009:LYS:HB2	1.86	0.58
3:D:1103:HIS:CD2	3:J:1462:LEU:H	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1123:PHE:CD2	3:D:1184:ARG:HG3	2.39	0.58
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.85	0.58
3:D:191:LEU:HD22	3:D:393:ILE:HG21	1.85	0.58
2:C:1089:VAL:HG11	2:C:1112:PHE:HE1	1.69	0.58
2:C:261:LEU:CD2	2:C:263:ASP:HB2	2.34	0.58
3:D:1031:ASN:HD21	3:D:1033:GLN:CD	2.08	0.58
3:D:44:LEU:HD22	3:D:544:TYR:HB3	1.86	0.58
3:D:805:ALA:O	3:D:832:ARG:HB2	2.04	0.58
3:D:804:MET:SD	3:D:831:GLY:HA3	2.44	0.58
1:B:179:PHE:HB2	1:B:197:LEU:HD12	1.86	0.57
2:C:545:ASN:HB3	2:C:583:LEU:CD1	2.34	0.57
2:C:650:LYS:O	2:C:652:GLY:N	2.37	0.57
3:D:1207:TYR:O	3:D:1209:LEU:N	2.37	0.57
3:D:783:ARG:O	3:D:784:ASP:CB	2.52	0.57
3:D:100:ALA:HA	3:D:513:ILE:HD13	1.85	0.57
3:D:154:THR:HG22	3:D:155:ASP:H	1.69	0.57
2:C:690:ILE:HG12	2:C:849:VAL:HG13	1.86	0.57
2:C:144:PRO:HA	2:C:163:ILE:HG22	1.86	0.57
2:C:719:PRO:HD2	2:C:761:PHE:HE1	1.66	0.57
3:D:102:ILE:HD11	3:D:579:ASP:HA	1.85	0.57
2:C:289:THR:HG23	2:C:302:VAL:HB	1.85	0.57
3:D:969:ARG:HD3	3:D:972:ARG:HD2	1.84	0.57
3:J:1423:GLY:O	3:J:1425:THR:N	2.37	0.57
1:B:176:ARG:HD3	1:B:200:TRP:CD1	2.40	0.57
2:C:39:ARG:HB3	2:C:45:GLN:HG3	1.86	0.57
3:D:1057:VAL:HG22	3:D:1069:GLU:HG2	1.87	0.57
3:D:613:ARG:HG3	3:D:613:ARG:O	2.05	0.57
3:D:656:PHE:HB3	3:D:694:VAL:HG11	1.85	0.57
3:D:971:LEU:O	3:D:974:ILE:HG22	2.05	0.57
3:D:1031:ASN:OD1	3:D:1034:GLN:NE2	2.38	0.56
2:C:1034:GLU:CD	3:D:1096:ARG:HH12	2.07	0.56
3:D:136:ASP:CB	3:D:137:PRO:CD	2.63	0.56
3:D:1197:ARG:HD2	3:J:1396:GLU:CB	2.33	0.56
3:D:653:PHE:O	3:D:656:PHE:HB2	2.04	0.56
2:C:788:THR:OG1	2:C:788:THR:O	2.19	0.56
2:C:881:ASN:HD22	2:C:881:ASN:N	2.04	0.56
3:D:407:VAL:HG13	3:D:422:ALA:HB2	1.87	0.56
2:C:52:PHE:O	2:C:54:ILE:N	2.38	0.56
3:D:657:LEU:HG	3:D:657:LEU:O	2.06	0.56
3:D:771:SER:HB2	3:D:778:LEU:HD22	1.86	0.56
3:J:1396:GLU:HG3	3:J:1396:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1258:ARG:HH21	3:J:1262:LEU:HD11	1.70	0.56
3:J:1310:ARG:HB3	3:J:1327:ARG:HD3	1.87	0.56
3:J:1412:LYS:HG3	3:J:1413:VAL:HG22	1.86	0.56
3:D:109:PRO:O	3:D:110:SER:HB2	2.05	0.56
3:D:631:ILE:HG23	3:D:745:MET:HB2	1.88	0.56
1:A:85:LEU:HA	1:A:124:ASN:HD21	1.70	0.56
2:C:57:GLY:O	2:C:58:ASP:HB2	2.05	0.56
3:D:1110:ALA:HA	3:D:1202:GLN:HB3	1.88	0.56
2:C:291:VAL:HG23	2:C:301:GLU:HG3	1.88	0.55
2:C:376:ARG:H	2:C:377:PRO:HD2	1.71	0.55
2:C:400:PRO:HG3	2:C:659:PRO:HD2	1.88	0.55
3:D:977:ALA:O	3:D:982:PHE:HB2	2.06	0.55
2:C:252:LYS:HZ2	2:C:298:PHE:HE1	1.53	0.55
2:C:487:THR:HB	2:C:490:GLU:H	1.70	0.55
2:C:569:VAL:O	2:C:571:LEU:HD12	2.07	0.55
2:C:289:THR:CG2	2:C:303:PHE:CE1	2.89	0.55
2:C:724:ARG:HG2	2:C:724:ARG:O	2.05	0.55
2:C:554:ASP:HB2	2:C:880:MET:HB2	1.89	0.55
2:C:903:SER:OG	2:C:908:GLY:HA3	2.06	0.55
2:C:394:PHE:HB2	5:C:1120:RFP:O8	2.06	0.55
2:C:1:MET:HG3	2:C:900:ARG:HE	1.71	0.55
2:C:631:SER:HB2	2:C:635:THR:HB	1.87	0.55
2:C:760:SER:H	2:C:788:THR:CG2	2.19	0.55
1:A:233:LEU:HD12	1:A:234:PRO:HD2	1.89	0.55
3:J:1277:ILE:HG13	3:J:1278:ASP:N	2.22	0.55
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.88	0.55
3:D:805:ALA:CB	3:D:832:ARG:H	2.07	0.55
2:C:399:ASN:HD21	2:C:401:LEU:HB3	1.72	0.54
3:D:900:ILE:HG21	3:D:902:MET:HE2	1.88	0.54
1:A:199:ILE:HG21	1:A:207:PRO:HA	1.89	0.54
1:A:215:VAL:HG23	1:B:222:LEU:HD22	1.88	0.54
1:A:53:VAL:HG21	1:A:82:LEU:O	2.06	0.54
2:C:26:TYR:HB2	2:C:121:MET:HE1	1.89	0.54
2:C:1101:THR:CG2	3:D:5:VAL:HG13	2.37	0.54
2:C:521:PRO:HB3	3:D:1068:LEU:CD2	2.38	0.54
1:A:73:GLU:HG3	1:A:130:ALA:HA	1.90	0.54
3:D:24:GLY:HA3	3:D:49:ILE:HB	1.89	0.54
4:K:41:GLU:HB3	4:K:42:PRO:CD	2.38	0.54
3:D:104:PHE:HD2	3:D:512:MET:SD	2.30	0.54
3:J:1465:ASN:HD21	3:J:1470:ARG:HH11	1.56	0.54
1:B:156:HIS:ND1	1:B:158:ILE:HG12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:546:LEU:HB3	2:C:565:GLN:HE22	1.72	0.54
3:D:212:ARG:HB3	3:D:386:HIS:HB2	1.90	0.54
1:A:201:THR:HG21	1:A:205:VAL:O	2.07	0.54
2:C:393:GLN:HG3	2:C:406:HIS:CE1	2.43	0.54
2:C:50:GLU:OE2	2:C:345:ARG:NE	2.37	0.54
3:D:860:LEU:HA	3:D:877:PRO:HB2	1.87	0.54
3:J:1258:ARG:HH11	3:J:1258:ARG:HG2	1.71	0.54
3:D:618:LEU:CD2	3:J:1463:LYS:HG3	2.37	0.54
3:D:551:ASN:HA	3:D:574:LEU:HD12	1.89	0.54
3:D:72:VAL:HG22	3:D:73:CYS:H	1.73	0.54
3:J:1258:ARG:NH1	3:J:1258:ARG:HG2	2.22	0.54
2:C:807:ARG:HA	2:C:821:GLU:HA	1.90	0.54
3:J:1278:ASP:N	3:J:1278:ASP:OD1	2.36	0.54
1:B:128:HIS:O	1:B:130:ALA:N	2.40	0.53
1:B:179:PHE:CB	1:B:197:LEU:HD12	2.38	0.53
3:J:1331:ASP:OD2	3:J:1334:GLN:HG3	2.08	0.53
1:A:38:ASN:H	1:A:39:PRO:HD2	1.74	0.53
2:C:1030:GLN:NE2	3:D:628:ARG:HG2	2.23	0.53
3:D:1109:GLU:HA	3:D:1217:ILE:HD13	1.90	0.53
1:A:44:LEU:HA	1:A:48:ILE:CD1	2.39	0.53
1:A:89:PHE:O	1:A:91:ASP:N	2.40	0.53
2:C:878:SER:HB2	3:D:1029:ARG:HD3	1.89	0.53
3:D:1161:GLU:CG	3:D:1164:ARG:HG3	2.32	0.53
2:C:710:ILE:HG21	2:C:756:VAL:HG11	1.89	0.53
4:K:26:ARG:HD2	4:K:29:GLN:HE21	1.73	0.53
2:C:831:ARG:O	2:C:832:LYS:HB2	2.08	0.53
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.44	0.53
2:C:565:GLN:HA	2:C:995:MET:HE1	1.90	0.53
3:D:584:ASN:HD21	3:D:591:VAL:HB	1.74	0.53
2:C:577:PRO:HA	2:C:671:ASN:HD21	1.72	0.53
2:C:602:GLU:O	2:C:613:VAL:HG23	2.08	0.53
3:D:1105:ILE:HG23	3:D:1199:GLY:HA2	1.90	0.53
3:D:160:GLU:HG2	3:D:165:LYS:HB2	1.91	0.53
2:C:1095:LEU:O	2:C:1096:ALA:HB3	2.09	0.53
3:D:638:LYS:HA	3:D:932:ASP:OD2	2.09	0.53
3:J:1353:GLN:HG2	3:J:1368:ILE:HD12	1.90	0.53
2:C:1006:HIS:HB3	2:C:1027:PHE:CG	2.44	0.53
3:D:483:HIS:N	3:D:484:PRO:HD3	2.24	0.53
3:D:907:GLU:HB2	3:D:1026:SER:HA	1.91	0.53
2:C:1020:PRO:HG2	3:D:622:ARG:HB2	1.90	0.53
2:C:324:ASP:C	2:C:326:ASP:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:631:SER:CB	2:C:635:THR:HB	2.39	0.53
2:C:841:ASN:ND2	2:C:845:ASN:H	2.07	0.53
2:C:902:ILE:HG22	2:C:902:ILE:O	2.08	0.53
3:D:792:ILE:CD1	3:D:881:LEU:HD23	2.34	0.53
3:D:1125:MET:HE3	3:D:1131:THR:O	2.09	0.52
3:D:543:LEU:HG	3:D:600:LEU:HD11	1.90	0.52
3:J:1349:VAL:HG22	3:J:1368:ILE:HG22	1.91	0.52
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.91	0.52
3:D:203:ALA:HA	3:D:394:LEU:O	2.10	0.52
1:A:198:ARG:O	1:A:199:ILE:CB	2.55	0.52
1:A:211:LEU:O	1:A:215:VAL:HG12	2.10	0.52
1:A:21:GLY:O	1:A:198:ARG:O	2.26	0.52
2:C:393:GLN:HB3	5:C:1120:RFP:O9	2.09	0.52
2:C:793:PRO:HG2	2:C:796:GLU:HB2	1.91	0.52
2:C:327:HIS:HD2	2:C:329:GLY:H	1.57	0.52
3:D:319:ALA:HB2	3:D:337:LEU:HD23	1.92	0.52
3:D:43:GLY:C	3:D:45:PHE:H	2.13	0.52
3:D:90:MET:HA	3:D:521:PRO:HD3	1.91	0.52
2:C:84:ARG:HA	2:C:131:GLY:HA2	1.90	0.52
2:C:650:LYS:HB2	2:C:653:ASP:HB2	1.89	0.52
3:D:97:THR:OG1	3:D:98:PRO:HD3	2.09	0.52
4:K:6:ILE:O	4:K:6:ILE:HD13	2.10	0.52
2:C:749:VAL:HG12	2:C:792:VAL:HG21	1.91	0.52
3:D:957:PRO:CD	3:D:1007:VAL:HG23	2.31	0.52
3:D:1106:VAL:O	3:D:1108:ARG:HG2	2.10	0.52
3:D:372:ASP:HB3	3:D:375:GLU:HB2	1.92	0.52
1:B:129:ILE:HG22	1:B:130:ALA:N	2.25	0.52
1:A:218:LEU:HD23	1:B:222:LEU:HD21	1.92	0.52
2:C:441:VAL:HG12	2:C:442:GLU:N	2.24	0.52
3:D:1197:ARG:CG	3:J:1396:GLU:HB3	2.40	0.52
1:A:86:VAL:HG21	1:A:202:ASP:HB2	1.91	0.52
1:A:20:TYR:C	1:A:20:TYR:HD2	2.13	0.52
2:C:369:PRO:C	2:C:371:LYS:H	2.12	0.52
2:C:605:LYS:HB2	2:C:612:ALA:HB3	1.91	0.52
2:C:631:SER:HB3	2:C:633:GLN:H	1.75	0.52
3:D:1208:ASP:C	3:D:1210:SER:N	2.63	0.52
3:D:129:PHE:O	3:D:131:LYS:N	2.42	0.52
3:D:190:GLU:HG2	3:D:196:VAL:HG13	1.91	0.52
2:C:271:GLU:HB3	2:C:464:LEU:CD2	2.40	0.51
2:C:967:PHE:HA	2:C:971:LYS:O	2.10	0.51
3:D:810:GLU:HG3	3:D:810:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1277:ILE:HG13	3:J:1278:ASP:H	1.74	0.51
4:K:38:THR:HG22	4:K:40:LEU:H	1.75	0.51
2:C:628:TYR:N	2:C:638:ASP:HB2	2.18	0.51
3:D:30:GLU:HG3	3:D:545:ARG:CD	2.28	0.51
2:C:843:HIS:CD2	2:C:884:GLN:HA	2.44	0.51
3:D:783:ARG:HH11	3:D:783:ARG:CG	2.15	0.51
1:B:26:GLU:CB	1:B:27:PRO:CD	2.68	0.51
2:C:272:ALA:O	2:C:276:LYS:N	2.40	0.51
1:B:59:GLU:HB2	1:B:139:TYR:HB3	1.92	0.51
2:C:216:ASP:O	2:C:219:GLN:HB2	2.10	0.51
2:C:436:GLY:O	2:C:459:ALA:HB2	2.11	0.51
3:D:44:LEU:CD2	3:D:544:TYR:HB3	2.41	0.51
3:D:631:ILE:CG2	3:D:745:MET:HB2	2.40	0.51
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.91	0.51
2:C:617:ASP:O	2:C:619:ARG:N	2.44	0.51
3:D:732:VAL:HG13	3:D:736:PHE:CD1	2.46	0.51
2:C:285:LEU:HD11	2:C:302:VAL:HG22	1.93	0.51
3:D:519:VAL:HG22	3:D:544:TYR:CE1	2.46	0.51
2:C:1101:THR:O	2:C:1108:PRO:HA	2.11	0.51
2:C:261:LEU:HG	2:C:263:ASP:H	1.75	0.51
3:D:1141:GLU:HA	3:D:1171:VAL:HG11	1.93	0.51
3:D:870:GLY:O	3:D:871:ARG:CB	2.52	0.51
1:A:20:TYR:C	1:A:20:TYR:CD2	2.84	0.51
1:B:82:LEU:O	1:B:85:LEU:HB3	2.11	0.50
3:D:139:GLY:HA2	3:D:452:ILE:HG22	1.93	0.50
3:D:886:VAL:HG11	3:D:900:ILE:HD11	1.92	0.50
2:C:1113:GLU:HG2	2:C:1113:GLU:O	2.11	0.50
3:J:1311:LEU:HD12	3:J:1313:VAL:H	1.76	0.50
2:C:134:ARG:NH1	2:C:392:SER:O	2.44	0.50
2:C:496:ILE:HG12	2:C:531:PHE:HB2	1.94	0.50
1:B:33:GLY:HA3	1:B:181:VAL:HG21	1.93	0.50
2:C:477:GLY:HA2	2:C:508:ILE:CD1	2.40	0.50
2:C:881:ASN:ND2	2:C:881:ASN:H	2.07	0.50
3:D:959:GLU:HB3	3:D:963:TYR:CD1	2.46	0.50
2:C:328:LEU:HB2	2:C:433:THR:CG2	2.41	0.50
2:C:874:LEU:HD21	3:D:787:LEU:HD22	1.92	0.50
3:D:100:ALA:HB1	3:D:105:VAL:HG21	1.93	0.50
1:B:32:PHE:HA	1:B:35:THR:HB	1.93	0.50
2:C:847:GLY:HA2	3:D:741:ASP:HA	1.94	0.50
3:J:1353:GLN:O	3:J:1357:ARG:HB2	2.12	0.50
2:C:1030:GLN:HB2	3:D:626:SER:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:GLU:O	2:C:175:GLU:HG3	2.12	0.50
2:C:202:TYR:HE1	2:C:300:ASP:OD1	1.94	0.50
2:C:886:LEU:HD23	3:D:951:ILE:HD12	1.93	0.50
2:C:448:ASN:O	2:C:449:ILE:C	2.50	0.49
3:D:107:ASP:CG	3:D:108:VAL:H	2.15	0.49
2:C:396:ASP:H	2:C:406:HIS:CD2	2.11	0.49
1:B:215:VAL:O	1:B:219:LYS:HB2	2.12	0.49
1:B:80:LEU:HD13	3:D:844:ALA:HA	1.95	0.49
2:C:1076:VAL:CB	2:C:1077:PRO:CD	2.79	0.49
2:C:673:LEU:HD23	2:C:867:VAL:HG12	1.95	0.49
2:C:707:ARG:HB2	2:C:826:PHE:HD2	1.74	0.49
3:D:12:LEU:HD21	3:D:104:PHE:HE2	1.77	0.49
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.94	0.49
3:D:666:PHE:O	3:D:667:ALA:HB3	2.11	0.49
2:C:1041:GLU:HG2	3:J:1472:ILE:CD1	2.40	0.49
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.26	0.49
3:D:219:GLU:HG2	3:D:271:TYR:OH	2.12	0.49
2:C:256:TYR:HD2	2:C:261:LEU:HD22	1.78	0.49
3:D:208:PRO:HG2	3:D:347:VAL:HG21	1.95	0.49
1:B:20:TYR:HA	1:B:199:ILE:O	2.12	0.49
2:C:110:GLU:HB2	2:C:369:PRO:HG2	1.94	0.49
2:C:760:SER:H	2:C:788:THR:HG21	1.76	0.49
3:D:660:LYS:O	3:D:664:LYS:HB2	2.13	0.49
1:A:58:ILE:HG23	1:A:140:MET:HG3	1.95	0.49
2:C:714:ASP:HA	2:C:719:PRO:HA	1.95	0.49
3:D:543:LEU:HD11	3:D:584:ASN:ND2	2.23	0.49
5:C:1120:RFP:N1	5:C:1120:RFP:H18C	2.27	0.49
2:C:650:LYS:C	2:C:652:GLY:N	2.66	0.49
2:C:637:PHE:CD1	2:C:659:PRO:HG3	2.38	0.49
3:D:191:LEU:HD13	3:D:393:ILE:HG21	1.95	0.49
3:D:450:TYR:N	3:D:450:TYR:CD1	2.80	0.49
1:B:186:LEU:N	1:B:189:ARG:O	2.31	0.49
2:C:260:LEU:O	2:C:261:LEU:HD23	2.12	0.49
2:C:436:GLY:HA3	2:C:469:THR:HG21	1.94	0.49
3:D:46:ASP:OD2	3:D:49:ILE:HG12	2.13	0.49
2:C:846:LYS:HG3	3:D:741:ASP:HB2	1.94	0.49
3:D:923:GLY:O	3:D:924:MET:C	2.51	0.49
3:J:1347:TYR:CZ	3:J:1351:GLU:HG3	2.48	0.49
2:C:263:ASP:CB	2:C:264:PRO:CD	2.74	0.49
3:J:1336:LEU:HG	3:J:1337:GLU:N	2.27	0.49
2:C:1059:ASP:CG	2:C:1083:GLU:HB2	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:416:ALA:HB1	3:D:417:PRO:HD2	1.94	0.48
3:D:540:LEU:HD11	3:D:603:LEU:HD13	1.95	0.48
3:J:1396:GLU:CG	3:J:1396:GLU:O	2.60	0.48
2:C:1006:HIS:O	3:D:627:GLY:HA3	2.13	0.48
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.48	0.48
3:D:759:ALA:HA	3:D:763:MET:HG3	1.95	0.48
3:D:84:ILE:HG13	3:D:84:ILE:H	1.45	0.48
3:J:1417:TRP:CD1	3:J:1417:TRP:C	2.86	0.48
2:C:442:GLU:O	2:C:442:GLU:CG	2.41	0.48
2:C:540:PHE:CZ	2:C:906:PHE:HE1	2.32	0.48
2:C:564:MET:O	2:C:567:GLN:N	2.46	0.48
2:C:546:LEU:HD11	2:C:666:LEU:HD23	1.94	0.48
3:D:963:TYR:CE2	3:D:1002:LYS:CB	2.92	0.48
2:C:632:ASN:HB3	2:C:633:GLN:HE21	1.76	0.48
2:C:953:VAL:HG22	2:C:966:LEU:HD13	1.96	0.48
3:D:1008:PHE:CZ	3:D:1032:PRO:HA	2.48	0.48
3:D:1014:ASN:O	3:D:1015:TYR:CB	2.62	0.48
3:D:19:ARG:NH2	3:D:515:GLU:HB3	2.29	0.48
2:C:139:GLN:NE2	2:C:334:ARG:HH21	2.11	0.48
3:D:1007:VAL:HG21	3:D:1039:CYS:HB2	1.95	0.48
3:D:1029:ARG:HG2	3:D:1029:ARG:NH1	2.27	0.48
3:D:1031:ASN:ND2	3:D:1033:GLN:HG2	2.22	0.48
1:A:62:LEU:H	1:A:62:LEU:HD12	1.79	0.48
2:C:351:LEU:HD11	2:C:373:VAL:HG22	1.95	0.48
1:B:118:ALA:C	1:B:120:VAL:H	2.16	0.48
2:C:147:TYR:O	2:C:148:PHE:HB2	2.13	0.48
2:C:230:ARG:HB3	2:C:233:GLU:HB2	1.96	0.48
2:C:25:SER:HA	2:C:28:LYS:HE2	1.96	0.48
3:J:1335:LEU:HD23	3:J:1344:VAL:CG2	2.43	0.48
2:C:544:THR:HG22	2:C:550:LEU:HD21	1.95	0.48
2:C:712:ALA:HB2	2:C:722:ILE:HD12	1.95	0.48
3:D:1060:SER:O	3:D:1062:ARG:N	2.47	0.48
3:D:465:LEU:HD13	3:D:509:PRO:O	2.14	0.48
3:D:85:VAL:HG11	3:D:89:ARG:HE	1.77	0.48
3:J:1307:LYS:C	3:J:1309:ALA:H	2.16	0.48
3:J:1382:THR:O	3:J:1416:ALA:HB3	2.13	0.48
2:C:109:LYS:HB3	2:C:109:LYS:HZ2	1.78	0.48
2:C:399:ASN:H	2:C:402:SER:HG	1.61	0.48
3:D:852:ALA:O	3:D:857:LEU:HB2	2.13	0.48
2:C:256:TYR:CD2	2:C:261:LEU:HD22	2.49	0.47
3:D:24:GLY:O	3:D:25:GLU:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:333:ILE:HD11	2:C:467:ILE:HD11	1.96	0.47
2:C:508:ILE:HD13	2:C:526:PRO:CB	2.40	0.47
3:D:262:LYS:N	3:D:269:LEU:O	2.47	0.47
3:D:368:VAL:H	3:D:377:VAL:HB	1.79	0.47
3:D:762:GLN:HE21	4:K:20:THR:HG21	1.79	0.47
2:C:684:PHE:CE2	2:C:685:GLU:HG2	2.49	0.47
2:C:815:LEU:HD13	2:C:822:VAL:HG23	1.95	0.47
3:D:396:VAL:C	3:D:398:ALA:H	2.16	0.47
1:B:118:ALA:C	1:B:120:VAL:N	2.67	0.47
2:C:177:GLU:C	2:C:179:SER:H	2.18	0.47
2:C:580:MET:HB3	2:C:584:GLU:OE2	2.14	0.47
2:C:732:ALA:HA	2:C:735:ARG:HD2	1.96	0.47
3:D:242:LEU:HD13	3:D:313:LEU:HD21	1.97	0.47
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.96	0.47
2:C:327:HIS:CD2	2:C:329:GLY:H	2.31	0.47
2:C:841:ASN:C	2:C:841:ASN:ND2	2.63	0.47
3:D:841:PHE:CB	3:D:864:VAL:CG1	2.92	0.47
1:A:143:ARG:NE	1:A:145:ASP:OD1	2.47	0.47
1:B:19:HIS:HA	1:B:201:THR:OG1	2.14	0.47
3:D:41:ARG:NH2	3:D:42:ASP:CG	2.68	0.47
3:D:804:MET:CG	3:D:805:ALA:H	2.26	0.47
3:J:1258:ARG:CG	3:J:1258:ARG:NH1	2.76	0.47
1:A:26:GLU:HB3	1:A:27:PRO:HD3	1.96	0.47
1:B:86:VAL:HB	1:B:123:MET:HB2	1.96	0.47
2:C:948:GLU:HB3	2:C:953:VAL:HB	1.96	0.47
3:D:1066:THR:O	3:D:1069:GLU:N	2.48	0.47
3:D:458:ALA:O	3:D:462:GLN:HB2	2.15	0.47
1:A:68:ILE:HB	1:A:71:VAL:CG2	2.45	0.47
1:B:176:ARG:HB3	1:B:200:TRP:CD1	2.49	0.47
2:C:193:LEU:HD22	2:C:197:LEU:HG	1.97	0.47
3:D:1211:MET:SD	4:K:16:LYS:HE3	2.54	0.47
2:C:549:PHE:HB3	2:C:552:HIS:HD2	1.80	0.47
3:D:73:CYS:HB2	3:D:77:GLY:HA2	1.97	0.47
2:C:396:ASP:HA	2:C:633:GLN:OE1	2.15	0.47
3:D:95:LEU:HD12	3:D:574:LEU:HD21	1.96	0.47
1:B:53:VAL:HG11	1:B:82:LEU:HD12	1.96	0.47
2:C:147:TYR:O	2:C:323:ASP:HB2	2.15	0.47
2:C:379:GLU:O	2:C:383:ARG:HB2	2.15	0.47
2:C:89:THR:HG22	2:C:91:GLN:HG3	1.96	0.47
3:D:813:LEU:HD11	3:D:839:LEU:HD22	1.97	0.47
3:D:762:GLN:NE2	4:K:20:THR:HG21	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:HD13	1:B:214:ALA:HB2	1.95	0.46
2:C:1071:ILE:HG13	3:D:670:VAL:HG11	1.97	0.46
2:C:160:ALA:HB2	2:C:310:LEU:HD13	1.96	0.46
2:C:857:ASP:O	2:C:858:MET:HB2	2.15	0.46
2:C:967:PHE:O	2:C:970:GLY:N	2.45	0.46
3:D:956:ILE:HG23	3:D:1039:CYS:O	2.15	0.46
3:D:202:VAL:O	3:D:395:VAL:HA	2.15	0.46
3:D:796:ARG:NH1	3:D:796:ARG:HG3	2.27	0.46
1:A:151:VAL:HA	1:A:152:PRO:HD3	1.77	0.46
3:D:25:GLU:HA	3:D:92:HIS:O	2.16	0.46
3:D:371:ILE:HG13	3:D:371:ILE:H	1.55	0.46
2:C:1046:ALA:HA	3:J:1472:ILE:HG22	1.98	0.46
2:C:256:TYR:HE2	2:C:261:LEU:HB3	1.79	0.46
3:D:1014:ASN:O	3:D:1015:TYR:CG	2.68	0.46
3:D:1031:ASN:HD21	3:D:1033:GLN:H	1.63	0.46
1:B:24:VAL:HG22	1:B:196:THR:HG23	1.97	0.46
2:C:1038:TRP:CD1	3:D:1099:VAL:HG11	2.49	0.46
2:C:502:PRO:HB2	2:C:509:ALA:HB3	1.98	0.46
2:C:856:GLU:H	2:C:856:GLU:CD	2.19	0.46
3:D:1015:TYR:N	3:D:1016:PRO:CD	2.78	0.46
3:D:179:VAL:HG21	3:D:191:LEU:HD23	1.96	0.46
3:D:705:ALA:CB	3:D:706:PRO:CD	2.64	0.46
1:A:34:VAL:HG12	1:A:179:PHE:HZ	1.80	0.46
1:B:132:LEU:H	1:B:132:LEU:HD22	1.80	0.46
3:D:121:THR:O	3:D:123:LEU:N	2.48	0.46
3:D:334:THR:C	3:D:335:LEU:HG	2.35	0.46
3:D:932:ASP:O	3:D:935:LYS:HB3	2.16	0.46
2:C:979:THR:O	2:C:981:GLU:N	2.49	0.46
3:D:456:MET:HG2	3:D:457:GLY:H	1.81	0.46
3:D:102:ILE:HD11	3:D:579:ASP:CA	2.45	0.46
3:D:668:PRO:HD2	3:D:669:ASN:H	1.81	0.46
2:C:26:TYR:HB2	2:C:121:MET:CE	2.46	0.46
3:D:530:VAL:O	3:D:532:GLY:N	2.49	0.46
3:D:583:ASP:O	3:D:586:ARG:HG2	2.16	0.46
3:D:646:LYS:HB2	3:D:688:TRP:CZ3	2.51	0.46
2:C:850:ALA:CB	3:D:632:VAL:HG22	2.46	0.46
3:D:284:LEU:HD13	3:D:305:ALA:HB2	1.98	0.46
2:C:1095:LEU:O	2:C:1096:ALA:CB	2.63	0.46
2:C:603:VAL:HG21	2:C:643:VAL:CG1	2.45	0.46
3:D:12:LEU:HD21	3:D:104:PHE:CE2	2.51	0.46
1:B:120:VAL:O	1:B:120:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1076:VAL:HG12	2:C:1077:PRO:HD3	1.97	0.46
3:D:186:VAL:CG1	3:D:187:LYS:N	2.79	0.46
1:B:65:PHE:CD1	3:D:813:LEU:HG	2.51	0.46
4:K:26:ARG:O	4:K:30:LEU:HB2	2.16	0.46
2:C:313:LEU:O	2:C:313:LEU:HG	2.16	0.45
3:D:367:ILE:HB	3:D:377:VAL:HG12	1.98	0.45
3:D:400:VAL:HG23	3:D:445:ARG:HB3	1.98	0.45
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.51	0.45
2:C:447:ALA:H	3:D:1085:ALA:HB1	1.80	0.45
2:C:524:VAL:HG13	2:C:528:GLU:HB2	1.97	0.45
2:C:494:TYR:HB3	2:C:530:GLU:HB2	1.98	0.45
3:D:1066:THR:O	3:D:1068:LEU:N	2.48	0.45
3:D:1111:ASP:C	3:D:1113:GLY:N	2.70	0.45
3:D:29:PRO:HB2	3:D:30:GLU:H	1.55	0.45
3:D:960:LYS:O	3:D:964:LEU:HB2	2.16	0.45
2:C:901:TYR:HE2	2:C:917:LEU:CD1	2.30	0.45
3:D:860:LEU:HD12	3:D:877:PRO:HB2	1.98	0.45
3:D:92:HIS:C	3:D:92:HIS:CD2	2.88	0.45
1:A:34:VAL:O	1:A:35:THR:C	2.54	0.45
1:B:216:ALA:O	1:B:220:GLU:HB2	2.17	0.45
2:C:582:GLY:O	2:C:584:GLU:N	2.50	0.45
2:C:575:GLN:NE2	2:C:670:GLN:HB3	2.25	0.45
2:C:971:LYS:HA	2:C:988:VAL:HA	1.99	0.45
3:D:101:HIS:C	3:D:101:HIS:CD2	2.90	0.45
3:D:827:ILE:O	3:D:836:VAL:HG13	2.16	0.45
2:C:399:ASN:ND2	2:C:401:LEU:HB3	2.31	0.45
3:D:112:ILE:HD11	3:D:512:MET:HB3	1.98	0.45
1:B:188:GLN:HG2	3:D:688:TRP:NE1	2.31	0.45
1:B:208:LEU:HG	1:B:212:ASN:ND2	2.32	0.45
1:B:55:SER:O	1:B:142:VAL:HA	2.17	0.45
2:C:210:GLU:O	2:C:308:ARG:HD2	2.16	0.45
2:C:21:ILE:HG13	2:C:21:ILE:H	1.46	0.45
2:C:363:SER:HA	2:C:364:PRO:HD3	1.80	0.45
2:C:966:LEU:HD11	2:C:986:PRO:HG3	1.99	0.45
3:D:39:PRO:HB3	3:D:45:PHE:HB3	1.98	0.45
3:D:835:SER:H	3:D:838:ARG:HG3	1.82	0.45
3:D:937:TYR:HA	3:D:940:THR:HG22	1.98	0.45
3:D:929:ARG:NH1	4:K:1:MET:HA	2.31	0.45
4:K:35:PHE:C	4:K:37:ASN:H	2.19	0.45
2:C:431:HIS:HB3	2:C:434:HIS:CE1	2.52	0.45
2:C:856:GLU:OE2	2:C:856:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:338:GLU:O	3:D:339:TRP:HB3	2.17	0.45
3:D:137:PRO:HD2	3:D:453:ASP:HB3	1.99	0.45
3:D:792:ILE:HG23	3:D:793:THR:HG23	1.98	0.45
2:C:1093:GLN:C	2:C:1095:LEU:H	2.20	0.45
2:C:261:LEU:CD2	2:C:263:ASP:CB	2.93	0.45
2:C:726:ILE:HB	2:C:729:LEU:HD22	1.99	0.45
3:D:602:SER:H	3:D:605:ASP:HB2	1.81	0.45
2:C:1034:GLU:CD	3:D:1096:ARG:NH1	2.68	0.45
2:C:198:ARG:HD2	2:C:198:ARG:HA	1.74	0.45
2:C:443:THR:OG1	2:C:444:PRO:HD2	2.17	0.45
2:C:809:GLY:O	2:C:810:ASP:O	2.35	0.45
3:D:178:LEU:HG	3:D:193:PRO:HD3	1.99	0.45
3:J:1457:ASP:O	3:J:1458:GLU:CB	2.61	0.45
2:C:901:TYR:HE2	2:C:917:LEU:HD11	1.82	0.45
3:D:186:VAL:HG12	3:D:187:LYS:N	2.32	0.45
3:D:875:THR:OG1	3:D:876:SER:N	2.48	0.45
3:D:1031:ASN:ND2	3:D:1033:GLN:H	2.15	0.44
3:D:1149:LEU:HD23	3:D:1187:PRO:O	2.16	0.44
3:D:136:ASP:CG	3:D:137:PRO:HD3	2.36	0.44
3:D:828:VAL:HG11	3:D:863:VAL:HG23	1.99	0.44
3:J:1258:ARG:NH2	3:J:1262:LEU:HD11	2.32	0.44
1:B:184:THR:N	1:B:192:LEU:O	2.45	0.44
2:C:110:GLU:HB2	2:C:369:PRO:CG	2.48	0.44
3:D:1117:TYR:HE2	3:D:1151:ARG:HE	1.66	0.44
3:D:729:HIS:CE1	3:D:731:LEU:HB2	2.51	0.44
2:C:194:VAL:HA	2:C:197:LEU:HD12	1.99	0.44
2:C:439:CYS:CB	2:C:541:SER:HB3	2.47	0.44
3:D:29:PRO:HB2	3:D:30:GLU:OE1	2.18	0.44
3:D:581:VAL:CG1	3:D:581:VAL:O	2.66	0.44
3:J:1272:ALA:HA	3:J:1326:THR:HG22	1.99	0.44
3:J:1342:GLU:H	3:J:1342:GLU:CD	2.21	0.44
1:B:17:GLY:O	1:B:18:ASP:CB	2.62	0.44
2:C:501:THR:HA	2:C:502:PRO:HD3	1.81	0.44
2:C:550:LEU:HB3	2:C:905:VAL:HG13	1.99	0.44
3:D:104:PHE:CD1	3:D:104:PHE:N	2.85	0.44
3:D:1174:LEU:HD13	3:D:1186:VAL:HG21	1.98	0.44
2:C:1018:GLN:HE21	2:C:1063:ARG:HH22	1.63	0.44
2:C:20:GLU:OE1	2:C:460:ARG:HD3	2.17	0.44
2:C:54:ILE:HD11	2:C:356:ARG:HG3	1.99	0.44
2:C:981:GLU:HB3	2:C:982:PRO:HD2	1.99	0.44
3:D:666:PHE:CD1	3:D:666:PHE:C	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:704:ARG:HG3	3:D:705:ALA:CB	2.48	0.44
3:J:1256:LEU:N	3:J:1257:PRO:CD	2.81	0.44
3:J:1314:LYS:HG2	3:J:1314:LYS:H	1.60	0.44
3:J:1376:LEU:O	3:J:1378:TYR:N	2.51	0.44
1:A:43:ILE:HG12	1:B:32:PHE:CE1	2.52	0.44
2:C:304:LEU:N	2:C:305:PRO:HD2	2.33	0.44
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.32	0.44
3:D:955:VAL:O	3:D:1039:CYS:HB3	2.17	0.44
3:D:764:LEU:HD23	3:D:767:HIS:CE1	2.52	0.44
3:D:923:GLY:O	3:D:925:GLU:N	2.51	0.44
3:D:98:PRO:O	3:D:99:ALA:HB2	2.18	0.44
3:J:1435:LEU:HD21	3:J:1468:LEU:HD21	1.99	0.44
1:A:218:LEU:O	1:A:222:LEU:HB2	2.17	0.44
1:B:52:ALA:CB	1:B:170:ILE:HD12	2.47	0.44
2:C:193:LEU:HD13	2:C:197:LEU:HD11	1.98	0.44
3:D:112:ILE:C	3:D:114:THR:H	2.21	0.44
3:D:996:TRP:CE2	3:D:1056:PRO:HG3	2.52	0.44
2:C:462:ASP:O	2:C:465:GLY:N	2.35	0.44
2:C:768:SER:O	2:C:771:GLU:HG3	2.17	0.44
2:C:809:GLY:O	2:C:810:ASP:C	2.57	0.44
2:C:8:ARG:HD2	2:C:8:ARG:HA	1.64	0.44
3:J:1413:VAL:HB	3:J:1415:VAL:H	1.82	0.44
3:J:1450:ALA:O	3:J:1453:ALA:O	2.36	0.44
2:C:1034:GLU:OE1	3:D:1096:ARG:NH1	2.51	0.44
2:C:393:GLN:OE1	5:C:1120:RFP:H343	2.18	0.44
2:C:52:PHE:CG	2:C:68:PHE:HB2	2.53	0.44
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.53	0.44
1:A:115:THR:HA	1:A:116:PRO:HD3	1.83	0.43
1:A:231:SER:HB3	1:B:15:THR:HG22	2.00	0.43
2:C:1097:LEU:N	2:C:1097:LEU:HD23	2.33	0.43
2:C:168:ARG:NH2	2:C:262:ALA:HB1	2.33	0.43
2:C:498:GLN:OE1	3:D:1068:LEU:HB2	2.18	0.43
3:D:1111:ASP:C	3:D:1113:GLY:H	2.21	0.43
3:D:771:SER:HA	3:D:772:PRO:HD3	1.87	0.43
2:C:274:ARG:O	2:C:278:GLU:N	2.44	0.43
2:C:601:GLY:N	2:C:649:VAL:HG22	2.19	0.43
3:D:111:LYS:HG2	3:J:1452:ILE:CD1	2.48	0.43
3:D:547:LEU:HD11	3:D:578:VAL:HG22	2.00	0.43
3:D:661:MET:HG2	3:D:666:PHE:CZ	2.52	0.43
3:D:937:TYR:O	3:D:938:GLY:C	2.57	0.43
2:C:699:PHE:O	2:C:701:THR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:751:PRO:HA	2:C:792:VAL:CG1	2.46	0.43
3:D:666:PHE:CD1	3:D:666:PHE:O	2.71	0.43
3:D:699:VAL:H	3:D:756:GLN:HE21	1.55	0.43
1:B:80:LEU:HB3	3:D:867:ARG:NH1	2.31	0.43
3:J:1269:LYS:O	3:J:1270:ALA:HB3	2.17	0.43
1:A:206:THR:O	1:A:207:PRO:C	2.57	0.43
2:C:1074:GLU:O	2:C:1076:VAL:N	2.45	0.43
3:D:1209:LEU:O	3:D:1209:LEU:HD12	2.18	0.43
3:D:770:LEU:HB3	3:D:775:GLY:O	2.17	0.43
3:D:806:PHE:HD2	3:D:810:GLU:HG2	1.84	0.43
3:J:1462:LEU:O	3:J:1463:LYS:C	2.56	0.43
4:K:33:HIS:O	4:K:35:PHE:N	2.51	0.43
2:C:131:GLY:O	2:C:132:ALA:O	2.36	0.43
2:C:508:ILE:HG13	2:C:508:ILE:H	1.41	0.43
2:C:436:GLY:HA2	2:C:538:GLN:O	2.19	0.43
3:D:951:ILE:HG12	3:D:1062:ARG:HD3	2.01	0.43
3:D:397:LYS:O	3:D:448:GLU:HB2	2.18	0.43
3:J:1460:ILE:CD1	3:J:1460:ILE:H	1.99	0.43
5:C:1120:RFP:H363	5:C:1120:RFP:C37	2.48	0.43
3:D:1060:SER:O	3:D:1063:GLU:N	2.51	0.43
3:D:661:MET:HE3	3:D:673:ALA:HB1	1.99	0.43
3:D:858:LEU:HD22	3:D:864:VAL:HG21	2.00	0.43
3:D:880:ILE:HD13	3:D:880:ILE:HA	1.76	0.43
3:D:974:ILE:HD11	3:D:991:GLN:HB3	1.99	0.43
3:D:999:THR:O	3:D:1003:VAL:HG23	2.19	0.43
3:J:1432:LYS:HD2	3:J:1432:LYS:N	2.34	0.43
2:C:289:THR:HG22	2:C:303:PHE:CD1	2.54	0.43
2:C:139:GLN:HB3	2:C:391:LEU:HD21	2.00	0.43
2:C:604:VAL:HG21	2:C:614:ARG:HB2	1.99	0.43
2:C:734:LEU:O	2:C:736:ASP:N	2.51	0.43
3:D:145:VAL:CB	3:D:146:PRO:CD	2.96	0.43
3:D:823:LEU:O	3:D:825:ALA:N	2.49	0.43
1:B:78:ILE:HG13	1:B:130:ALA:HB2	2.00	0.43
2:C:140:ILE:CD1	2:C:331:ARG:HH21	2.31	0.43
2:C:475:LYS:O	2:C:476:ASN:C	2.56	0.43
2:C:968:ASP:C	2:C:970:GLY:H	2.22	0.43
2:C:99:GLN:HB3	2:C:109:LYS:HG3	2.01	0.43
3:D:195:VAL:HG12	3:D:196:VAL:N	2.34	0.43
3:D:773:ALA:HA	3:J:1367:HIS:NE2	2.34	0.43
2:C:462:ASP:O	2:C:463:ALA:C	2.57	0.43
3:D:41:ARG:HH22	3:D:48:ARG:NE	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:732:VAL:CG1	3:D:736:PHE:HD1	2.32	0.43
3:D:810:GLU:O	3:D:811:GLU:C	2.58	0.43
1:A:44:LEU:HD23	1:A:48:ILE:HD13	2.01	0.43
2:C:257:LEU:C	2:C:259:GLY:H	2.19	0.43
3:D:1060:SER:O	3:D:1061:PHE:C	2.57	0.43
4:K:31:LEU:HD13	4:K:60:ALA:HB2	2.01	0.43
1:B:101:LEU:HD21	1:B:109:VAL:HG11	2.00	0.42
2:C:143:SER:HA	2:C:144:PRO:HD2	1.87	0.42
2:C:317:VAL:HB	2:C:320:HIS:CD2	2.54	0.42
2:C:42:VAL:N	2:C:46:ALA:HB2	2.34	0.42
2:C:599:GLU:O	2:C:600:ASP:C	2.57	0.42
2:C:841:ASN:HD21	2:C:845:ASN:H	1.65	0.42
3:D:1099:VAL:O	3:D:1103:HIS:HB3	2.19	0.42
3:D:638:LYS:H	3:D:641:GLN:HE21	1.66	0.42
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.42
3:D:790:TYR:CE2	3:D:794:GLN:HG3	2.54	0.42
2:C:886:LEU:HD23	3:D:951:ILE:CD1	2.48	0.42
1:A:23:PHE:O	1:A:196:THR:HA	2.18	0.42
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.79	0.42
2:C:124:ASP:HA	2:C:592:LEU:HD12	2.01	0.42
2:C:272:ALA:HA	2:C:275:TYR:HB3	2.01	0.42
3:D:804:MET:O	3:D:805:ALA:O	2.37	0.42
1:A:186:LEU:O	1:A:188:GLN:N	2.52	0.42
1:B:93:LYS:HA	1:B:93:LYS:HD2	1.76	0.42
2:C:790:LEU:O	2:C:791:ARG:HB2	2.19	0.42
2:C:876:VAL:H	2:C:877:PRO:CD	2.32	0.42
3:D:45:PHE:CZ	3:D:527:MET:HB2	2.55	0.42
3:D:12:LEU:HD23	3:D:507:ASN:HD22	1.84	0.42
3:D:49:ILE:HG13	3:D:50:PHE:N	2.34	0.42
1:A:90:LEU:HG	1:A:119:ASP:C	2.39	0.42
2:C:879:ARG:H	2:C:879:ARG:CD	2.24	0.42
3:D:1205:TYR:CE1	3:D:1221:VAL:CG1	2.98	0.42
3:D:704:ARG:HG3	3:D:705:ALA:HB3	2.02	0.42
3:D:883:ALA:HB2	3:D:902:MET:CE	2.49	0.42
1:A:96:SER:HB3	1:A:145:ASP:HA	2.02	0.42
1:B:115:THR:HA	1:B:116:PRO:HD3	1.86	0.42
2:C:1088:LEU:O	2:C:1089:VAL:C	2.57	0.42
2:C:144:PRO:HG3	2:C:165:LEU:HG	2.00	0.42
2:C:20:GLU:OE1	2:C:460:ARG:CD	2.67	0.42
2:C:513:VAL:HG12	2:C:524:VAL:HG12	2.00	0.42
2:C:958:SER:HB3	2:C:961:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1211:MET:O	3:D:1213:ARG:HG3	2.19	0.42
2:C:1012:PRO:HG2	2:C:1024:LYS:H	1.85	0.42
2:C:141:HIS:CE1	2:C:334:ARG:HG3	2.55	0.42
2:C:568:ALA:HB2	2:C:995:MET:HE3	2.01	0.42
2:C:717:LEU:HD13	2:C:762:LYS:HA	2.01	0.42
3:D:1209:LEU:HG	3:D:1211:MET:CE	2.50	0.42
3:D:710:ARG:N	3:D:1227:GLU:OE1	2.51	0.42
4:K:33:HIS:O	4:K:34:ARG:C	2.58	0.42
2:C:1030:GLN:HB2	3:D:626:SER:CB	2.49	0.42
2:C:11:GLU:H	2:C:11:GLU:HG2	1.63	0.42
2:C:390:GLN:HE21	2:C:414:GLY:HA2	1.85	0.42
2:C:439:CYS:HB2	2:C:541:SER:HB3	2.01	0.42
2:C:856:GLU:N	2:C:856:GLU:CD	2.72	0.42
3:D:205:TYR:CD2	3:D:387:LEU:HD12	2.55	0.42
3:D:237:ARG:HB3	3:D:238:PRO:HD2	2.01	0.42
1:A:179:PHE:HB3	1:A:197:LEU:HD23	2.00	0.42
2:C:711:GLU:HG2	2:C:822:VAL:HG22	2.01	0.42
3:D:1123:PHE:HA	3:D:1134:LEU:HA	2.01	0.42
3:D:137:PRO:HD2	3:D:453:ASP:O	2.19	0.42
3:J:1335:LEU:HD23	3:J:1344:VAL:HG23	2.02	0.42
1:A:184:THR:HB	1:A:194:LYS:HB2	2.01	0.42
2:C:30:LEU:HA	2:C:44:ILE:HD12	2.02	0.42
2:C:42:VAL:HA	2:C:46:ALA:HB2	2.01	0.42
2:C:78:PHE:CZ	2:C:812:GLY:HA3	2.55	0.42
3:D:1205:TYR:CD2	3:D:1215:VAL:HG21	2.51	0.42
3:D:538:SER:HB3	3:D:541:ASN:ND2	2.35	0.42
1:A:225:PHE:CD2	1:B:11:PHE:CE1	2.97	0.41
2:C:193:LEU:HD12	2:C:307:LEU:HD13	2.02	0.41
2:C:324:ASP:C	2:C:326:ASP:N	2.73	0.41
2:C:343:GLN:HA	2:C:346:VAL:HG23	2.02	0.41
2:C:753:ASP:O	2:C:791:ARG:HA	2.20	0.41
3:D:1019:PRO:C	3:D:1023:MET:HE2	2.41	0.41
3:D:169:TYR:HB2	3:D:393:ILE:HG22	2.02	0.41
3:D:548:ILE:H	3:D:548:ILE:HG13	1.69	0.41
3:J:1434:TRP:CE2	3:J:1435:LEU:HD13	2.55	0.41
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.91	0.41
1:B:202:ASP:OD2	1:B:204:SER:N	2.53	0.41
2:C:42:VAL:CA	2:C:46:ALA:HB2	2.49	0.41
2:C:762:LYS:HB3	2:C:764:GLU:OE1	2.20	0.41
2:C:971:LYS:HB3	2:C:986:PRO:HB2	2.02	0.41
3:D:1053:PHE:CE1	3:D:1072:ILE:HG22	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1202:GLN:O	3:D:1204:CYS:O	2.38	0.41
3:D:26:VAL:HG13	3:D:93:ILE:HG12	2.02	0.41
3:D:709:HIS:O	3:D:710:ARG:C	2.57	0.41
3:D:964:LEU:O	3:D:968:ASP:HB2	2.20	0.41
3:D:732:VAL:CG1	3:D:736:PHE:CD1	3.04	0.41
1:B:85:LEU:HA	1:B:124:ASN:HD21	1.85	0.41
1:B:36:LEU:O	1:B:39:PRO:HD2	2.20	0.41
1:B:5:LYS:HB3	1:B:6:LEU:H	1.74	0.41
2:C:10:ARG:HD2	2:C:10:ARG:HA	1.85	0.41
2:C:853:LEU:HA	2:C:854:PRO:HD2	1.90	0.41
3:D:237:ARG:HB3	3:D:238:PRO:CD	2.50	0.41
3:D:247:GLU:HA	3:D:248:PRO:HD3	1.95	0.41
4:K:68:LEU:HA	4:K:73:LEU:HD12	2.03	0.41
2:C:551:GLU:HB2	2:C:552:HIS:CD2	2.56	0.41
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.35	0.41
2:C:807:ARG:HG2	2:C:807:ARG:H	1.75	0.41
2:C:755:LEU:HD22	2:C:825:VAL:HG11	2.02	0.41
3:D:161:LEU:HD23	3:D:452:ILE:HD13	2.01	0.41
1:B:25:LEU:HD23	1:B:28:LEU:HD11	2.03	0.41
2:C:1005:MET:HB2	3:D:629:SER:CB	2.47	0.41
2:C:375:SER:OG	2:C:375:SER:O	2.30	0.41
2:C:474:VAL:HG12	2:C:479:VAL:HA	2.02	0.41
2:C:755:LEU:HG	2:C:792:VAL:HG23	2.02	0.41
2:C:87:ASP:OD2	2:C:824:ARG:NH2	2.49	0.41
3:D:416:ALA:O	3:D:419:ASP:HB2	2.21	0.41
3:D:466:LYS:HA	3:D:510:GLU:HG2	2.02	0.41
3:D:23:TYR:CE2	3:D:89:ARG:HD3	2.55	0.41
4:K:6:ILE:HA	4:K:9:LEU:HD12	2.03	0.41
1:A:34:VAL:HG12	1:A:179:PHE:CZ	2.55	0.41
1:A:43:ILE:HD12	1:A:218:LEU:HB2	2.03	0.41
1:A:90:LEU:N	1:A:90:LEU:HD23	2.35	0.41
2:C:94:LEU:HD21	2:C:344:PHE:HZ	1.86	0.41
3:D:1004:THR:OG1	3:D:1036:ARG:HD3	2.21	0.41
3:D:335:LEU:O	3:D:337:LEU:HG	2.21	0.41
3:D:474:GLU:HG3	3:D:503:LEU:HD13	2.02	0.41
3:D:731:LEU:HA	3:D:731:LEU:HD23	1.92	0.41
3:D:794:GLN:HG2	3:D:905:PRO:HB3	2.03	0.41
3:D:920:LEU:HA	3:D:920:LEU:HD13	1.89	0.41
4:K:15:SER:O	4:K:16:LYS:C	2.59	0.41
1:A:77:GLU:HG3	2:C:640:ARG:NH2	2.35	0.41
2:C:1006:HIS:HB3	2:C:1027:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:154:ARG:NH1	2:C:176:VAL:O	2.54	0.41
2:C:721:ARG:O	2:C:758:ARG:HA	2.21	0.41
2:C:549:PHE:CE2	2:C:909:ALA:HB3	2.55	0.41
3:D:801:GLY:O	3:D:802:ALA:HB2	2.21	0.41
3:D:804:MET:SD	3:D:805:ALA:N	2.86	0.41
2:C:889:HIS:HE1	3:D:951:ILE:H	1.67	0.41
3:D:968:ASP:O	3:D:971:LEU:HB3	2.21	0.41
5:C:1120:RFP:O4	5:C:1120:RFP:O12	2.39	0.41
3:D:1147:ARG:CB	3:D:1188:VAL:HG21	2.40	0.41
3:D:520:LEU:HD23	3:D:525:ARG:HG2	2.02	0.41
3:D:884:ARG:O	3:D:888:GLU:N	2.38	0.41
5:C:1120:RFP:H24C	5:C:1120:RFP:H342	1.91	0.41
2:C:710:ILE:HG21	2:C:756:VAL:CG1	2.51	0.41
3:D:1118:ILE:CG1	3:D:1190:SER:HB3	2.51	0.41
3:D:223:LEU:HG	3:D:224:ARG:N	2.34	0.41
3:D:285:PRO:HG2	3:D:311:LEU:HD22	2.02	0.41
3:D:804:MET:SD	3:D:805:ALA:HB2	2.61	0.41
1:A:192:LEU:O	2:C:938:LYS:NZ	2.54	0.40
1:A:86:VAL:O	1:A:86:VAL:CG2	2.68	0.40
1:B:176:ARG:HB3	1:B:200:TRP:HB2	2.03	0.40
2:C:17:PRO:HD2	2:C:20:GLU:CG	2.47	0.40
3:D:1219:GLU:HG2	3:D:1221:VAL:HG22	2.04	0.40
3:D:396:VAL:C	3:D:398:ALA:N	2.75	0.40
3:J:1363:LEU:HD12	3:J:1363:LEU:O	2.21	0.40
2:C:177:GLU:HG2	2:C:177:GLU:H	1.66	0.40
2:C:261:LEU:CG	2:C:263:ASP:HB2	2.51	0.40
2:C:941:LYS:O	2:C:942:GLU:C	2.59	0.40
2:C:995:MET:HB2	2:C:995:MET:HE2	1.88	0.40
3:D:508:ARG:C	3:D:510:GLU:H	2.25	0.40
3:J:1306:PRO:O	3:J:1307:LYS:CB	2.69	0.40
3:D:618:LEU:HD22	3:J:1463:LYS:HE3	2.03	0.40
4:K:44:GLU:OE2	4:K:72:ARG:NH2	2.54	0.40
2:C:906:PHE:O	2:C:907:ASP:HB2	2.21	0.40
2:C:911:GLU:HA	2:C:914:ILE:HD12	2.02	0.40
3:D:191:LEU:HD13	3:D:393:ILE:CG2	2.51	0.40
3:J:1262:LEU:HD12	3:J:1262:LEU:HA	1.78	0.40
4:K:41:GLU:O	4:K:42:PRO:C	2.60	0.40
3:D:1174:LEU:HD23	3:D:1174:LEU:HA	1.83	0.40
3:D:118:LEU:O	3:D:119:SER:C	2.60	0.40
3:D:855:HIS:HB2	3:D:857:LEU:HD22	2.02	0.40
2:C:368:THR:HB	2:C:369:PRO:CD	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:431:HIS:HB3	2:C:434:HIS:ND1	2.37	0.40
3:D:1063:GLU:HG3	3:D:1063:GLU:H	1.67	0.40
3:D:1072:ILE:HG12	3:D:1072:ILE:H	1.66	0.40
3:D:58:CYS:HB3	3:D:59:ALA:H	1.61	0.40
3:D:637:LEU:HB2	3:D:641:GLN:HB2	2.04	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%)	173 (76%)	38 (17%)	17 (8%)	1	7
1	B	223/314 (71%)	177 (79%)	31 (14%)	15 (7%)	1	8
2	C	1112/1119 (99%)	871 (78%)	153 (14%)	88 (8%)	1	6
3	D	1236/1524 (81%)	968 (78%)	187 (15%)	81 (7%)	1	8
3	J	247/1524 (16%)	194 (78%)	40 (16%)	13 (5%)	2	12
4	K	93/99 (94%)	74 (80%)	8 (9%)	11 (12%)	0	2
All	All	3139/4894 (64%)	2457 (78%)	457 (15%)	225 (7%)	1	7

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	161	ARG
1	A	203	GLY
1	B	18	ASP
1	B	26	GLU
1	B	129	ILE
2	C	9	ILE

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Mol	Chain	Res	Type
2	C	42	VAL
2	C	132	ALA
2	C	148	PHE
2	C	183	THR
2	C	213	ALA
2	C	264	PRO
2	C	283	VAL
2	C	315	ALA
2	C	394	PHE
2	C	422	ARG
2	C	449	ILE
2	C	564	MET
2	C	735	ARG
2	C	762	LYS
2	C	764	GLU
2	C	780	GLU
2	C	907	ASP
2	C	936	VAL
2	C	1046	ALA
2	C	1077	PRO
2	C	1096	ALA
2	C	1097	LEU
2	C	1106	ASP
3	D	41	ARG
3	D	99	ALA
3	D	110	SER
3	D	130	ASN
3	D	136	ASP
3	D	531	ASP
3	D	666	PHE
3	D	679	ARG
3	D	795	VAL
3	D	802	ALA
3	D	805	ALA
3	D	827	ILE
3	D	860	LEU
3	D	871	ARG
3	D	875	THR
3	D	924	MET
3	D	1061	PHE
3	D	1067	VAL
3	D	1197	ARG

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Mol	Chain	Res	Type
3	D	1208	ASP
3	J	1377	LYS
3	J	1424	VAL
3	J	1455	LYS
4	K	2	ALA
4	K	34	ARG
4	K	41	GLU
4	K	42	PRO
1	A	59	GLU
1	A	126	ASP
1	A	139	TYR
1	A	157	GLY
1	A	187	GLY
1	A	199	ILE
1	B	30	ARG
1	B	61	VAL
1	B	119	ASP
2	C	64	LEU
2	C	111	ASP
2	C	242	LEU
2	C	257	LEU
2	C	284	GLY
2	C	316	GLY
2	C	433	THR
2	C	476	ASN
2	C	563	ASN
2	C	583	LEU
2	C	618	GLY
2	C	699	PHE
2	C	716	LYS
2	C	740	GLU
2	C	811	PRO
2	C	1060	ILE
2	C	1076	VAL
2	C	1078	GLU
3	D	25	GLU
3	D	30	GLU
3	D	32	ILE
3	D	97	THR
3	D	119	SER
3	D	132	TYR
3	D	321	GLU

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Mol	Chain	Res	Type
3	D	427	VAL
3	D	643	GLY
3	D	705	ALA
3	D	775	GLY
3	D	783	ARG
3	D	784	ASP
3	D	791	TYR
3	D	824	ASN
3	D	925	GLU
3	D	1181	GLY
3	D	1205	TYR
4	K	16	LYS
4	K	35	PHE
1	A	20	TYR
1	A	27	PRO
1	A	74	ASP
1	A	165	ILE
1	B	5	LYS
1	B	6	LEU
1	B	20	TYR
2	C	112	GLU
2	C	247	PRO
2	C	290	LEU
2	C	292	ARG
2	C	293	PHE
2	C	325	ILE
2	C	463	ALA
2	C	538	GLN
2	C	651	LYS
2	C	659	PRO
2	C	700	TYR
2	C	739	GLU
2	C	788	THR
3	D	24	GLY
3	D	29	PRO
3	D	44	LEU
3	D	50	PHE
3	D	69	GLU
3	D	349	PRO
3	D	397	LYS
3	D	546	ARG
3	D	600	LEU

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Mol	Chain	Res	Type
3	D	610	LYS
3	D	629	SER
3	D	758	GLU
3	D	804	MET
3	D	823	LEU
3	D	1015	TYR
3	D	1091	SER
3	J	1270	ALA
3	J	1307	LYS
4	K	80	VAL
1	A	118	ALA
1	A	136	GLY
1	A	234	PRO
1	B	17	GLY
1	B	75	VAL
1	B	104	GLU
1	B	118	ALA
2	C	8	ARG
2	C	41	ASN
2	C	66	LEU
2	C	178	ALA
2	C	252	LYS
2	C	258	PHE
2	C	619	ARG
2	C	652	GLY
2	C	858	MET
2	C	980	GLY
2	C	1075	ASP
2	C	1110	ASP
3	D	39	PRO
3	D	57	GLU
3	D	58	CYS
3	D	117	ASP
3	D	122	GLU
3	D	207	PHE
3	D	594	PRO
3	D	613	ARG
3	D	667	ALA
3	D	680	GLN
3	D	800	LYS
3	J	1315	ASP
3	J	1458	GLU

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Mol	Chain	Res	Type
4	K	38	THR
1	A	38	ASN
1	B	133	GLU
2	C	53	PRO
2	C	261	LEU
2	C	262	ALA
2	C	336	VAL
2	C	376	ARG
2	C	629	ALA
2	C	685	GLU
2	C	810	ASP
2	C	821	GLU
2	C	1005	MET
2	C	1099	VAL
3	D	72	VAL
3	D	109	PRO
3	D	120	ALA
3	D	127	LEU
3	D	389	GLU
3	D	521	PRO
3	D	587	ARG
3	D	621	LYS
3	D	668	PRO
3	D	1026	SER
3	J	1285	GLU
3	J	1383	ASP
3	J	1405	GLU
3	J	1415	VAL
4	K	4	PRO
4	K	93	TYR
2	C	876	VAL
2	C	959	PRO
2	C	1113	GLU
3	D	522	PRO
3	D	1079	LYS
3	J	1327	ARG
3	J	1408	ILE
2	C	645	VAL
2	C	1079	PRO
3	D	828	VAL
1	B	120	VAL
2	C	248	PRO

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Mol	Chain	Res	Type
3	D	885	ILE
3	D	1080	GLY
4	K	94	PRO
2	C	186	VAL
2	C	263	ASP
3	D	1019	PRO
2	C	548	PRO
2	C	194	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/270 (70%)	132 (70%)	57 (30%)	0	1
1	B	191/270 (71%)	130 (68%)	61 (32%)	0	1
2	C	889/936 (95%)	610 (69%)	279 (31%)	0	1
3	D	992/1281 (77%)	666 (67%)	326 (33%)	0	1
3	J	191/1281 (15%)	125 (65%)	66 (35%)	0	1
4	K	75/88 (85%)	59 (79%)	16 (21%)	1	4
All	All	2527/4126 (61%)	1722 (68%)	805 (32%)	0	1

All (805) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	19	HIS
1	A	20	TYR
1	A	24	VAL
1	A	29	GLU
1	A	32	PHE
1	A	34	VAL
1	A	40	LEU
1	A	44	LEU
1	A	53	VAL

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Mol	Chain	Res	Type
1	A	54	THR
1	A	55	SER
1	A	58	ILE
1	A	59	GLU
1	A	62	LEU
1	A	64	GLU
1	A	67	THR
1	A	72	LYS
1	A	74	ASP
1	A	77	GLU
1	A	79	ILE
1	A	83	LYS
1	A	86	VAL
1	A	87	VAL
1	A	90	LEU
1	A	94	MET
1	A	101	LEU
1	A	107	LYS
1	A	108	GLU
1	A	114	PHE
1	A	115	THR
1	A	119	ASP
1	A	120	VAL
1	A	126	ASP
1	A	127	LEU
1	A	133	GLU
1	A	134	GLU
1	A	143	ARG
1	A	144	VAL
1	A	145	ASP
1	A	151	VAL
1	A	159	LYS
1	A	160	ASP
1	A	161	ARG
1	A	167	VAL
1	A	172	SER
1	A	176	ARG
1	A	183	ASP
1	A	186	LEU
1	A	190	THR
1	A	196	THR
1	A	198	ARG

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Mol	Chain	Res	Type
1	A	201	THR
1	A	215	VAL
1	A	222	LEU
1	A	229	GLU
1	A	231	SER
1	B	4	SER
1	B	5	LYS
1	B	7	LYS
1	B	10	VAL
1	B	19	HIS
1	B	26	GLU
1	B	41	ARG
1	B	42	ARG
1	B	44	LEU
1	B	51	THR
1	B	55	SER
1	B	56	VAL
1	B	59	GLU
1	B	60	ASP
1	B	61	VAL
1	B	62	LEU
1	B	64	GLU
1	B	66	SER
1	B	67	THR
1	B	78	ILE
1	B	79	ILE
1	B	82	LEU
1	B	88	ARG
1	B	93	LYS
1	B	96	SER
1	B	97	THR
1	B	101	LEU
1	B	104	GLU
1	B	110	ARG
1	B	119	ASP
1	B	126	ASP
1	B	132	LEU
1	B	134	GLU
1	B	137	LYS
1	B	138	LEU
1	B	145	ASP
1	B	146	ARG

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Mol	Chain	Res	Type
1	B	148	VAL
1	B	151	VAL
1	B	159	LYS
1	B	160	ASP
1	B	162	ILE
1	B	165	ILE
1	B	167	VAL
1	B	170	ILE
1	B	171	PHE
1	B	174	VAL
1	B	175	ARG
1	B	176	ARG
1	B	180	GLN
1	B	182	GLU
1	B	183	ASP
1	B	184	THR
1	B	186	LEU
1	B	188	GLN
1	B	189	ARG
1	B	198	ARG
1	B	213	GLN
1	B	217	ILE
1	B	219	LYS
1	B	220	GLU
2	C	1	MET
2	C	4	LYS
2	C	8	ARG
2	C	9	ILE
2	C	10	ARG
2	C	11	GLU
2	C	12	VAL
2	C	20	GLU
2	C	21	ILE
2	C	26	TYR
2	C	28	LYS
2	C	30	LEU
2	C	33	ASP
2	C	34	VAL
2	C	42	VAL
2	C	50	GLU
2	C	51	THR
2	C	52	PHE

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Mol	Chain	Res	Type
2	C	55	GLU
2	C	56	GLU
2	C	58	ASP
2	C	73	ILE
2	C	79	SER
2	C	80	GLN
2	C	88	LEU
2	C	94	LEU
2	C	95	TYR
2	C	97	ARG
2	C	98	LEU
2	C	101	ILE
2	C	103	LYS
2	C	104	ASP
2	C	105	THR
2	C	111	ASP
2	C	113	VAL
2	C	115	LEU
2	C	118	LEU
2	C	120	LEU
2	C	124	ASP
2	C	138	SER
2	C	139	GLN
2	C	142	ARG
2	C	144	PRO
2	C	149	THR
2	C	159	ILE
2	C	161	SER
2	C	165	LEU
2	C	167	LYS
2	C	175	GLU
2	C	177	GLU
2	C	179	SER
2	C	181	VAL
2	C	184	MET
2	C	193	LEU
2	C	194	VAL
2	C	195	LEU
2	C	196	LEU
2	C	198	ARG
2	C	204	GLN
2	C	207	LEU

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Mol	Chain	Res	Type
2	C	210	GLU
2	C	211	LEU
2	C	214	TYR
2	C	216	ASP
2	C	218	VAL
2	C	219	GLN
2	C	222	LEU
2	C	227	LEU
2	C	229	MET
2	C	232	GLU
2	C	237	ARG
2	C	241	LEU
2	C	242	LEU
2	C	246	ASP
2	C	250	LYS
2	C	258	PHE
2	C	261	LEU
2	C	271	GLU
2	C	275	TYR
2	C	283	VAL
2	C	285	LEU
2	C	290	LEU
2	C	293	PHE
2	C	295	ASP
2	C	299	LYS
2	C	304	LEU
2	C	308	ARG
2	C	309	TYR
2	C	310	LEU
2	C	314	THR
2	C	321	GLU
2	C	322	VAL
2	C	323	ASP
2	C	335	THR
2	C	345	ARG
2	C	348	LEU
2	C	351	LEU
2	C	371	LYS
2	C	375	SER
2	C	376	ARG
2	C	378	LEU
2	C	382	LEU

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Mol	Chain	Res	Type
2	C	389	SER
2	C	391	LEU
2	C	393	GLN
2	C	395	LYS
2	C	397	GLU
2	C	399	ASN
2	C	402	SER
2	C	403	SER
2	C	404	LEU
2	C	407	LYS
2	C	408	ARG
2	C	413	LEU
2	C	425	PHE
2	C	429	ASP
2	C	432	ARG
2	C	433	THR
2	C	442	GLU
2	C	443	THR
2	C	445	GLU
2	C	449	ILE
2	C	453	THR
2	C	454	SER
2	C	460	ARG
2	C	462	ASP
2	C	469	THR
2	C	472	ARG
2	C	473	ARG
2	C	476	ASN
2	C	478	VAL
2	C	480	THR
2	C	481	GLU
2	C	487	THR
2	C	493	ARG
2	C	495	THR
2	C	498	GLN
2	C	500	ASN
2	C	508	ILE
2	C	513	VAL
2	C	514	VAL
2	C	516	ARG
2	C	517	ARG
2	C	518	ARG

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Mol	Chain	Res	Type
2	C	520	GLU
2	C	523	ILE
2	C	535	SER
2	C	541	SER
2	C	542	LEU
2	C	544	THR
2	C	545	ASN
2	C	546	LEU
2	C	550	LEU
2	C	556	ASN
2	C	557	ARG
2	C	559	LEU
2	C	573	ARG
2	C	579	VAL
2	C	585	GLU
2	C	589	ARG
2	C	595	LEU
2	C	598	GLU
2	C	599	GLU
2	C	603	VAL
2	C	607	ASP
2	C	609	THR
2	C	610	ARG
2	C	613	VAL
2	C	620	LEU
2	C	625	LEU
2	C	626	ARG
2	C	627	ARG
2	C	630	ARG
2	C	631	SER
2	C	632	ASN
2	C	633	GLN
2	C	635	THR
2	C	637	PHE
2	C	638	ASP
2	C	650	LYS
2	C	655	LEU
2	C	657	ASP
2	C	671	ASN
2	C	674	VAL
2	C	688	ILE
2	C	692	GLU

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Mol	Chain	Res	Type
2	C	698	ASP
2	C	699	PHE
2	C	704	HIS
2	C	707	ARG
2	C	713	ARG
2	C	714	ASP
2	C	715	THR
2	C	720	GLU
2	C	722	ILE
2	C	728	HIS
2	C	731	GLU
2	C	735	ARG
2	C	737	LEU
2	C	758	ARG
2	C	770	GLU
2	C	771	GLU
2	C	772	ARG
2	C	774	LEU
2	C	784	ASP
2	C	785	VAL
2	C	788	THR
2	C	790	LEU
2	C	796	GLU
2	C	805	ARG
2	C	806	LEU
2	C	807	ARG
2	C	815	LEU
2	C	820	ARG
2	C	830	LYS
2	C	835	VAL
2	C	841	ASN
2	C	846	LYS
2	C	848	VAL
2	C	853	LEU
2	C	855	VAL
2	C	856	GLU
2	C	857	ASP
2	C	861	LEU
2	C	871	LEU
2	C	878	SER
2	C	879	ARG
2	C	881	ASN

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Mol	Chain	Res	Type
2	C	882	LEU
2	C	886	LEU
2	C	902	ILE
2	C	916	GLU
2	C	917	LEU
2	C	918	LEU
2	C	928	LYS
2	C	939	ARG
2	C	946	ARG
2	C	952	LEU
2	C	958	SER
2	C	961	GLU
2	C	963	LEU
2	C	964	LYS
2	C	969	LEU
2	C	972	VAL
2	C	979	THR
2	C	1000	MET
2	C	1001	VAL
2	C	1002	GLU
2	C	1005	MET
2	C	1006	HIS
2	C	1010	THR
2	C	1015	LEU
2	C	1018	GLN
2	C	1021	LEU
2	C	1024	LYS
2	C	1027	PHE
2	C	1030	GLN
2	C	1031	ARG
2	C	1035	MET
2	C	1040	LEU
2	C	1052	MET
2	C	1053	LEU
2	C	1057	SER
2	C	1058	ASP
2	C	1061	GLU
2	C	1063	ARG
2	C	1068	GLN
2	C	1071	ILE
2	C	1072	LYS
2	C	1076	VAL

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Mol	Chain	Res	Type
2	C	1080	SER
2	C	1085	PHE
2	C	1091	GLU
2	C	1095	LEU
2	C	1097	LEU
2	C	1101	THR
2	C	1102	LEU
2	C	1106	ASP
2	C	1113	GLU
3	D	9	ARG
3	D	12	LEU
3	D	16	GLU
3	D	17	LYS
3	D	20	SER
3	D	23	TYR
3	D	28	LYS
3	D	30	GLU
3	D	34	TYR
3	D	36	THR
3	D	41	ARG
3	D	44	LEU
3	D	46	ASP
3	D	53	ILE
3	D	54	LYS
3	D	55	ASP
3	D	58	CYS
3	D	64	LYS
3	D	66	GLN
3	D	73	CYS
3	D	74	GLU
3	D	75	ARG
3	D	81	THR
3	D	83	SER
3	D	84	ILE
3	D	85	VAL
3	D	87	ARG
3	D	90	MET
3	D	92	HIS
3	D	93	ILE
3	D	95	LEU
3	D	97	THR
3	D	102	ILE

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Mol	Chain	Res	Type
3	D	106	LYS
3	D	110	SER
3	D	111	LYS
3	D	114	THR
3	D	115	LEU
3	D	118	LEU
3	D	119	SER
3	D	121	THR
3	D	125	GLN
3	D	128	TYR
3	D	129	PHE
3	D	149	LYS
3	D	151	GLN
3	D	156	GLU
3	D	162	ARG
3	D	166	GLN
3	D	168	THR
3	D	184	GLU
3	D	189	GLN
3	D	196	VAL
3	D	198	ARG
3	D	204	LEU
3	D	206	ARG
3	D	209	ARG
3	D	214	ASP
3	D	218	LYS
3	D	220	ARG
3	D	224	ARG
3	D	227	LEU
3	D	233	LYS
3	D	234	GLU
3	D	240	GLU
3	D	261	LEU
3	D	263	ASP
3	D	266	GLU
3	D	273	ARG
3	D	277	GLU
3	D	278	VAL
3	D	279	VAL
3	D	284	LEU
3	D	293	VAL
3	D	297	ILE

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Mol	Chain	Res	Type
3	D	299	GLU
3	D	300	VAL
3	D	308	LYS
3	D	310	LEU
3	D	313	LEU
3	D	315	ARG
3	D	316	HIS
3	D	318	THR
3	D	322	VAL
3	D	325	GLU
3	D	329	ASP
3	D	331	VAL
3	D	333	LEU
3	D	335	LEU
3	D	347	VAL
3	D	354	ILE
3	D	357	GLU
3	D	360	LYS
3	D	365	GLU
3	D	371	ILE
3	D	375	GLU
3	D	387	LEU
3	D	389	GLU
3	D	392	SER
3	D	393	ILE
3	D	396	VAL
3	D	400	VAL
3	D	404	GLU
3	D	405	ASP
3	D	407	VAL
3	D	411	THR
3	D	414	ARG
3	D	415	VAL
3	D	434	ARG
3	D	435	VAL
3	D	436	GLU
3	D	441	ARG
3	D	445	ARG
3	D	450	TYR
3	D	455	ARG
3	D	462	GLN
3	D	463	GLU

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Mol	Chain	Res	Type
3	D	465	LEU
3	D	470	LEU
3	D	471	GLU
3	D	474	GLU
3	D	478	LEU
3	D	482	LYS
3	D	486	ARG
3	D	494	LYS
3	D	496	LEU
3	D	500	ARG
3	D	502	PHE
3	D	503	LEU
3	D	508	ARG
3	D	514	LEU
3	D	515	GLU
3	D	524	LEU
3	D	525	ARG
3	D	527	MET
3	D	537	THR
3	D	540	LEU
3	D	542	ASP
3	D	544	TYR
3	D	546	ARG
3	D	547	LEU
3	D	549	ASN
3	D	550	ARG
3	D	555	LYS
3	D	557	LEU
3	D	558	LEU
3	D	560	GLN
3	D	566	ILE
3	D	568	ARG
3	D	569	ASN
3	D	570	GLU
3	D	572	ARG
3	D	575	GLN
3	D	587	ARG
3	D	598	ARG
3	D	600	LEU
3	D	603	LEU
3	D	607	LEU
3	D	608	SER

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Mol	Chain	Res	Type
3	D	610	LYS
3	D	613	ARG
3	D	615	ARG
3	D	616	GLN
3	D	619	LEU
3	D	622	ARG
3	D	632	VAL
3	D	637	LEU
3	D	646	LYS
3	D	647	ARG
3	D	648	MET
3	D	652	LEU
3	D	654	LYS
3	D	664	LYS
3	D	666	PHE
3	D	668	PRO
3	D	669	ASN
3	D	670	VAL
3	D	671	LYS
3	D	676	MET
3	D	679	ARG
3	D	680	GLN
3	D	681	ARG
3	D	683	ILE
3	D	684	LYS
3	D	689	ASP
3	D	691	LEU
3	D	695	ILE
3	D	700	VAL
3	D	704	ARG
3	D	709	HIS
3	D	710	ARG
3	D	711	LEU
3	D	713	ILE
3	D	717	GLN
3	D	721	VAL
3	D	727	GLN
3	D	732	VAL
3	D	734	GLU
3	D	752	SER
3	D	754	PHE
3	D	763	MET

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Mol	Chain	Res	Type
3	D	771	SER
3	D	778	LEU
3	D	780	LYS
3	D	782	SER
3	D	785	ILE
3	D	791	TYR
3	D	792	ILE
3	D	794	GLN
3	D	795	VAL
3	D	797	LYS
3	D	798	GLU
3	D	804	MET
3	D	810	GLU
3	D	811	GLU
3	D	813	LEU
3	D	817	GLU
3	D	827	ILE
3	D	832	ARG
3	D	836	VAL
3	D	838	ARG
3	D	840	LYS
3	D	842	VAL
3	D	847	ASP
3	D	853	VAL
3	D	857	LEU
3	D	858	LEU
3	D	859	ASP
3	D	860	LEU
3	D	863	VAL
3	D	867	ARG
3	D	869	LEU
3	D	872	ARG
3	D	876	SER
3	D	880	ILE
3	D	888	GLU
3	D	893	GLU
3	D	902	MET
3	D	903	ASP
3	D	904	VAL
3	D	907	GLU
3	D	914	LEU
3	D	920	LEU

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Mol	Chain	Res	Type
3	D	921	ARG
3	D	922	LEU
3	D	925	GLU
3	D	927	THR
3	D	931	LEU
3	D	936	TYR
3	D	941	LEU
3	D	943	THR
3	D	944	THR
3	D	948	THR
3	D	956	ILE
3	D	960	LYS
3	D	968	ASP
3	D	969	ARG
3	D	974	ILE
3	D	975	GLU
3	D	979	GLU
3	D	980	MET
3	D	986	ARG
3	D	988	ARG
3	D	993	ILE
3	D	994	GLN
3	D	995	LEU
3	D	1001	GLU
3	D	1007	VAL
3	D	1009	LYS
3	D	1014	ASN
3	D	1020	LEU
3	D	1029	ARG
3	D	1031	ASN
3	D	1033	GLN
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	1063	GLU
3	D	1065	LEU
3	D	1067	VAL
3	D	1072	ILE
3	D	1073	SER

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Mol	Chain	Res	Type
3	D	1078	ARG
3	D	1083	ASP
3	D	1086	LEU
3	D	1090	ASP
3	D	1097	LYS
3	D	1098	LEU
3	D	1101	VAL
3	D	1104	GLU
3	D	1118	ILE
3	D	1119	SER
3	D	1126	ASP
3	D	1127	GLU
3	D	1129	THR
3	D	1135	ARG
3	D	1137	ARG
3	D	1138	SER
3	D	1141	GLU
3	D	1142	SER
3	D	1147	ARG
3	D	1148	VAL
3	D	1151	ARG
3	D	1152	GLU
3	D	1159	ARG
3	D	1161	GLU
3	D	1179	GLU
3	D	1182	GLU
3	D	1184	ARG
3	D	1188	VAL
3	D	1189	ARG
3	D	1190	SER
3	D	1196	THR
3	D	1200	VAL
3	D	1201	CYS
3	D	1207	TYR
3	D	1209	LEU
3	D	1216	SER
3	D	1219	GLU
3	D	1228	SER
3	D	1231	GLU
3	D	1234	THR
3	D	1238	MET
3	J	1253	THR

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Mol	Chain	Res	Type
3	J	1254	GLN
3	J	1258	ARG
3	J	1262	LEU
3	J	1264	GLU
3	J	1266	ARG
3	J	1269	LYS
3	J	1274	ILE
3	J	1275	SER
3	J	1278	ASP
3	J	1290	LEU
3	J	1304	LYS
3	J	1307	LYS
3	J	1310	ARG
3	J	1311	LEU
3	J	1312	LEU
3	J	1314	LYS
3	J	1315	ASP
3	J	1317	ASP
3	J	1319	VAL
3	J	1325	LEU
3	J	1326	THR
3	J	1327	ARG
3	J	1336	LEU
3	J	1339	LYS
3	J	1342	GLU
3	J	1344	VAL
3	J	1346	ARG
3	J	1348	LEU
3	J	1359	GLN
3	J	1366	LYS
3	J	1376	LEU
3	J	1379	VAL
3	J	1381	VAL
3	J	1386	ASP
3	J	1387	SER
3	J	1389	LEU
3	J	1399	ASP
3	J	1400	VAL
3	J	1403	LEU
3	J	1412	LYS
3	J	1413	VAL
3	J	1417	TRP

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Mol	Chain	Res	Type
3	J	1421	LEU
3	J	1424	VAL
3	J	1429	LEU
3	J	1430	SER
3	J	1431	THR
3	J	1432	LYS
3	J	1434	TRP
3	J	1435	LEU
3	J	1439	SER
3	J	1442	ASN
3	J	1456	LYS
3	J	1458	GLU
3	J	1459	LEU
3	J	1460	ILE
3	J	1463	LYS
3	J	1468	LEU
3	J	1470	ARG
3	J	1472	ILE
3	J	1476	THR
3	J	1482	ARG
3	J	1487	VAL
3	J	1495	ILE
3	J	1500	LYS
4	K	6	ILE
4	K	30	LEU
4	K	31	LEU
4	K	38	THR
4	K	40	LEU
4	K	49	ARG
4	K	50	THR
4	K	56	ASP
4	K	61	VAL
4	K	66	LYS
4	K	69	LEU
4	K	72	ARG
4	K	78	ASN
4	K	79	LEU
4	K	89	MET
4	K	93	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	221	HIS
1	A	227	ASN
1	B	19	HIS
1	B	180	GLN
1	B	212	ASN
1	B	213	GLN
1	B	221	HIS
1	B	223	ASN
2	C	139	GLN
2	C	141	HIS
2	C	219	GLN
2	C	320	HIS
2	C	327	HIS
2	C	390	GLN
2	C	399	ASN
2	C	406	HIS
2	C	431	HIS
2	C	565	GLN
2	C	575	GLN
2	C	623	HIS
2	C	632	ASN
2	C	633	GLN
2	C	639	GLN
2	C	647	GLN
2	C	671	ASN
2	C	765	GLN
2	C	841	ASN
2	C	845	ASN
2	C	881	ASN
2	C	884	GLN
2	C	889	HIS
2	C	1018	GLN
2	C	1030	GLN
3	D	101	HIS
3	D	507	ASN
3	D	552	ASN
3	D	616	GLN
3	D	640	HIS
3	D	641	GLN
3	D	669	ASN
3	D	717	GLN
3	D	724	GLN

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Mol	Chain	Res	Type
3	D	756	GLN
3	D	897	GLN
3	D	1031	ASN
3	D	1034	GLN
3	D	1037	GLN
3	D	1103	HIS
3	D	1195	GLN
3	J	1374	GLN
3	J	1465	ASN
4	K	29	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	RFP	C	1120	-	63,63,63	1.50	10 (15%)	94,94,94	2.35	20 (21%)

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	RFP	C	1120	-	-	12/60/85/85	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1120	RFP	C43-N2	5.95	1.44	1.27
5	C	1120	RFP	O7-C35	4.43	1.45	1.35
5	C	1120	RFP	O2-C8	-3.20	1.24	1.35
5	C	1120	RFP	O5-C29	3.11	1.47	1.39
5	C	1120	RFP	N3-N2	-3.06	1.31	1.39
5	C	1120	RFP	C3-C43	2.75	1.51	1.46
5	C	1120	RFP	C10-C9	2.69	1.49	1.42
5	C	1120	RFP	C8-C9	2.64	1.51	1.43
5	C	1120	RFP	C5-C10	2.60	1.48	1.43
5	C	1120	RFP	C8-C7	2.30	1.49	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1120	RFP	C42-N4-C39	13.50	128.40	109.52
5	C	1120	RFP	C3-C43-N2	-7.93	110.01	121.54
5	C	1120	RFP	C41-N3-C40	5.83	128.93	113.74
5	C	1120	RFP	C40-C39-N4	4.80	116.23	110.80
5	C	1120	RFP	C38-N4-C39	4.23	116.98	110.66
5	C	1120	RFP	O7-C35-C36	4.12	118.67	111.09
5	C	1120	RFP	C41-C42-N4	4.03	115.35	110.80
5	C	1120	RFP	C12-O5-C29	3.80	127.24	117.84
5	C	1120	RFP	C30-C16-C17	-3.41	115.17	123.42
5	C	1120	RFP	C42-C41-N3	3.39	116.01	110.51
5	C	1120	RFP	C25-O7-C35	-3.00	113.08	117.72
5	C	1120	RFP	C39-C40-N3	2.80	115.07	110.51
5	C	1120	RFP	O3-C6-C7	2.78	125.92	121.14
5	C	1120	RFP	C38-N4-C42	2.65	114.62	110.66
5	C	1120	RFP	C17-C18-C19	-2.55	118.33	124.53
5	C	1120	RFP	C43-N2-N3	2.49	123.93	120.43
5	C	1120	RFP	O7-C35-O8	-2.28	118.44	122.96
5	C	1120	RFP	C4-C3-C43	-2.09	114.02	116.52
5	C	1120	RFP	C2-C3-C4	2.09	120.54	119.20
5	C	1120	RFP	O4-C11-C12	2.06	124.76	120.56

There are no chirality outliers.

All (12) torsion outliers are listed below:

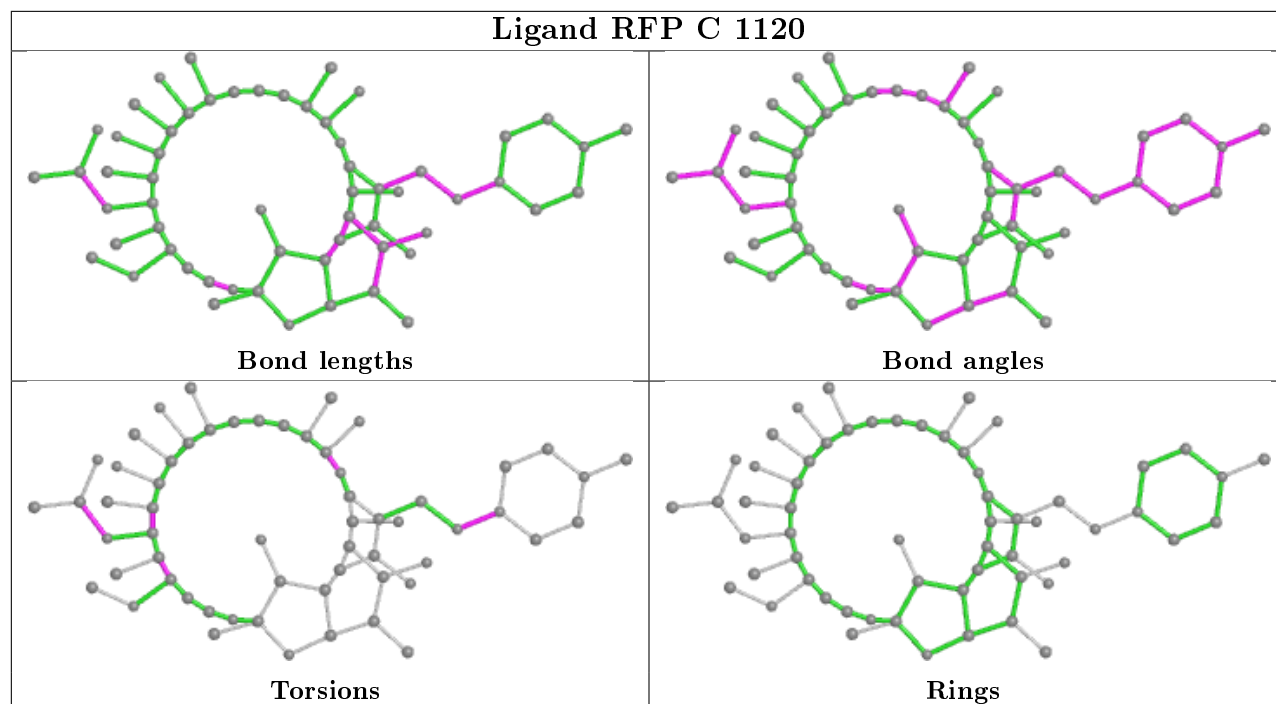
Mol	Chain	Res	Type	Atoms
5	C	1120	RFP	C16-C15-N1-C2
5	C	1120	RFP	O11-C15-N1-C2
5	C	1120	RFP	C36-C35-O7-C25
5	C	1120	RFP	C43-N2-N3-C40
5	C	1120	RFP	C43-N2-N3-C41
5	C	1120	RFP	O8-C35-O7-C25
5	C	1120	RFP	C33-C24-C25-O7
5	C	1120	RFP	C33-C24-C25-C26
5	C	1120	RFP	C23-C24-C25-O7
5	C	1120	RFP	C23-C24-C25-C26
5	C	1120	RFP	C34-C26-C27-O6
5	C	1120	RFP	C34-C26-C27-C28

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1120	RFP	10	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	230/314 (73%)	-0.03	14 (6%)	21 20	17, 38, 68, 98	0
1	B	225/314 (71%)	0.09	17 (7%)	13 13	24, 48, 73, 76	0
2	C	1114/1119 (99%)	0.02	51 (4%)	32 30	17, 44, 76, 93	0
3	D	1238/1524 (81%)	0.54	190 (15%)	2 2	15, 49, 87, 130	0
3	J	249/1524 (16%)	0.19	18 (7%)	15 15	17, 45, 114, 122	0
4	K	95/99 (95%)	0.51	15 (15%)	2 2	20, 59, 140, 154	0
All	All	3151/4894 (64%)	0.25	305 (9%)	7 8	15, 46, 85, 154	0

All (305) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	349	PRO	11.9
3	J	1403	LEU	11.7
3	D	57	GLU	11.1
3	D	256	SER	10.0
3	D	191	LEU	9.5
3	D	200	ASP	7.8
3	D	342	PRO	7.6
2	C	270	GLY	7.4
3	D	276	GLU	7.3
1	A	235	THR	7.2
3	D	807	ALA	7.0
3	D	808	THR	7.0
3	D	175	VAL	6.7
2	C	1023	GLY	6.4
3	J	1402	ALA	6.2
3	D	482	LYS	6.1
2	C	60	GLY	6.0
2	C	269	LEU	5.9
3	D	194	GLY	5.8

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Mol	Chain	Res	Type	RSRZ
3	D	179	VAL	5.7
3	D	348	ALA	5.6
2	C	318	PRO	5.5
2	C	59	LYS	5.5
4	K	53	GLY	5.5
3	D	425	GLY	5.4
3	J	1407	LEU	5.3
1	A	234	PRO	5.2
3	D	172	PRO	5.2
3	D	66	GLN	5.1
3	D	56	TYR	5.0
3	J	1408	ILE	5.0
3	D	192	ALA	5.0
3	D	535	PHE	5.0
3	D	75	ARG	4.9
3	D	199	MET	4.9
3	D	595	GLY	4.9
3	D	168	THR	4.8
3	D	566	ILE	4.8
3	D	350	HIS	4.7
3	D	422	ALA	4.7
3	D	70	GLY	4.7
3	J	1287	GLU	4.7
2	C	1022	GLY	4.6
3	D	479	GLU	4.6
3	D	39	PRO	4.6
3	D	534	ARG	4.6
3	D	379	ALA	4.6
3	D	55	ASP	4.6
3	D	58	CYS	4.5
3	D	588	GLY	4.5
4	K	54	LEU	4.5
3	D	340	THR	4.5
3	D	564	GLU	4.5
3	D	481	MET	4.4
3	D	371	ILE	4.4
3	D	370	ALA	4.4
3	D	69	GLU	4.4
3	D	375	GLU	4.4
3	D	71	LYS	4.4
3	D	299	GLU	4.3
3	D	82	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
3	D	424	GLY	4.3
3	J	1414	PRO	4.3
3	D	488	ARG	4.2
2	C	111	ASP	4.2
2	C	62	GLY	4.2
3	D	1240	THR	4.1
3	D	565	ILE	4.1
3	D	238	PRO	4.1
3	D	67	ARG	4.1
3	D	63	TYR	4.1
4	K	93	TYR	4.1
3	D	362	GLN	4.0
2	C	61	LYS	4.0
3	D	587	ARG	4.0
2	C	294	GLU	4.0
3	D	165	LYS	4.0
3	D	568	ARG	4.0
3	D	483	HIS	4.0
3	D	406	ASP	4.0
3	D	244	GLU	3.9
2	C	1102	LEU	3.9
3	D	341	GLU	3.9
3	D	367	ILE	3.9
3	D	596	SER	3.9
3	D	178	LEU	3.8
3	D	167	GLU	3.8
3	D	201	GLY	3.8
1	A	233	LEU	3.8
3	D	166	GLN	3.8
1	B	4	SER	3.8
3	D	177	ALA	3.8
3	D	563	PRO	3.7
3	D	405	ASP	3.7
3	D	384	VAL	3.7
3	J	1286	GLY	3.7
3	D	52	PRO	3.7
3	D	809	PRO	3.7
3	D	164	GLY	3.7
2	C	739	GLU	3.7
2	C	508	ILE	3.7
3	J	1308	ASP	3.7
3	D	986	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
3	D	560	GLN	3.6
3	D	982	PHE	3.6
1	B	91	ASP	3.6
3	D	196	VAL	3.6
3	D	478	LEU	3.6
3	D	174	GLY	3.6
3	J	1498	ALA	3.5
3	D	306	GLU	3.5
3	D	529	GLN	3.5
2	C	58	ASP	3.5
3	D	214	ASP	3.5
3	D	423	ASP	3.4
4	K	1	MET	3.4
3	D	188	GLY	3.4
3	D	831	GLY	3.4
3	D	326	GLU	3.4
2	C	55	GLU	3.4
3	D	528	VAL	3.4
3	D	365	GLU	3.4
1	A	203	GLY	3.4
3	D	680	GLN	3.4
3	D	198	ARG	3.4
3	D	532	GLY	3.4
3	D	170	PRO	3.3
3	D	275	GLU	3.3
3	D	137	PRO	3.3
2	C	295	ASP	3.3
4	K	55	TYR	3.2
3	J	1496	GLU	3.2
3	D	80	VAL	3.2
2	C	954	SER	3.2
2	C	1021	LEU	3.1
3	J	1497	GLU	3.1
3	D	381	ALA	3.1
3	D	132	TYR	3.1
2	C	1026	GLN	3.1
3	D	215	TYR	3.0
4	K	48	MET	3.0
3	D	185	VAL	3.0
3	D	980	MET	3.0
3	D	811	GLU	3.0
3	D	598	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	504	GLU	3.0
3	J	1404	ASN	3.0
3	D	234	GLU	3.0
2	C	1068	GLN	3.0
3	D	527	MET	2.9
3	D	41	ARG	2.9
3	D	561	GLY	2.9
3	D	277	GLU	2.9
3	D	318	THR	2.9
3	D	157	GLU	2.9
3	D	163	TYR	2.9
3	D	592	THR	2.8
3	J	1406	ARG	2.8
3	D	380	GLU	2.8
2	C	1	MET	2.8
1	A	20	TYR	2.8
3	D	421	LEU	2.8
3	D	533	GLY	2.8
3	D	208	PRO	2.8
3	D	487	ALA	2.8
1	A	159	LYS	2.8
3	D	1079	LYS	2.8
2	C	271	GLU	2.8
2	C	620	LEU	2.8
1	A	19	HIS	2.8
1	B	228	PRO	2.7
1	A	16	GLN	2.7
3	D	420	VAL	2.7
3	D	821	VAL	2.7
3	D	404	GLU	2.7
2	C	264	PRO	2.7
3	D	1129	THR	2.7
1	A	155	ARG	2.7
4	K	94	PRO	2.7
1	B	6	LEU	2.7
2	C	284	GLY	2.7
3	D	31	THR	2.6
2	C	154	ARG	2.6
4	K	84	ARG	2.6
1	B	89	PHE	2.6
4	K	95	THR	2.6
3	D	390	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	256	TYR	2.6
3	D	173	ALA	2.6
3	D	246	SER	2.6
3	D	679	ARG	2.6
3	D	402	PRO	2.6
3	D	820	GLU	2.6
3	D	183	GLU	2.6
3	D	195	VAL	2.6
1	B	5	LYS	2.6
3	D	338	GLU	2.6
3	D	383	GLY	2.6
2	C	2	GLU	2.5
4	K	2	ALA	2.5
1	B	94	MET	2.5
3	D	40	GLU	2.5
3	D	203	ALA	2.5
1	B	132	LEU	2.5
3	D	308	LYS	2.5
3	D	452	ILE	2.5
1	B	157	GLY	2.5
3	J	1411	GLY	2.5
3	D	74	GLU	2.5
1	A	230	ALA	2.5
3	D	401	TYR	2.5
3	D	983	LEU	2.5
3	D	119	SER	2.5
3	J	1500	LYS	2.5
1	B	133	GLU	2.5
3	D	979	GLU	2.5
4	K	50	THR	2.5
3	D	1239	ARG	2.5
2	C	153	ALA	2.4
1	B	159	LYS	2.4
3	D	300	VAL	2.4
2	C	282	GLY	2.4
2	C	1106	ASP	2.4
3	D	154	THR	2.4
3	D	263	ASP	2.4
3	D	78	VAL	2.4
3	D	366	LYS	2.3
3	D	474	GLU	2.3
3	D	407	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	268	ASP	2.3
3	D	190	GLU	2.3
3	D	169	TYR	2.3
3	D	315	ARG	2.3
3	D	432	TYR	2.3
2	C	248	PRO	2.3
3	J	1501	GLU	2.3
4	K	52	GLU	2.3
2	C	1105	LYS	2.3
3	D	153	LEU	2.3
3	D	427	VAL	2.3
3	D	981	GLY	2.3
4	K	86	GLN	2.3
2	C	615	TYR	2.3
1	B	14	THR	2.3
2	C	762	LYS	2.3
3	D	138	LYS	2.3
3	D	307	GLY	2.3
2	C	216	ASP	2.3
3	D	590	PRO	2.3
3	D	531	ASP	2.3
3	D	1115	THR	2.3
3	D	558	LEU	2.3
3	J	1413	VAL	2.3
1	B	134	GLU	2.2
3	D	832	ARG	2.2
2	C	246	ASP	2.2
3	D	42	ASP	2.2
3	D	16	GLU	2.2
1	B	158	ILE	2.2
1	A	18	ASP	2.2
3	D	176	ASP	2.2
3	D	511	TRP	2.2
3	D	207	PHE	2.2
3	D	1051	GLU	2.2
3	D	248	PRO	2.2
2	C	56	GLU	2.2
3	D	30	GLU	2.2
3	D	79	GLU	2.2
3	D	216	LEU	2.1
3	J	1389	LEU	2.1
2	C	958	SER	2.1

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Mol	Chain	Res	Type	RSRZ
4	K	5	GLY	2.1
2	C	959	PRO	2.1
2	C	223	ASP	2.1
1	A	185	ARG	2.1
4	K	47	LYS	2.1
3	D	567	ILE	2.1
2	C	107	LEU	2.1
2	C	155	PRO	2.1
3	D	83	SER	2.1
3	D	597	GLU	2.1
2	C	454	SER	2.1
3	D	72	VAL	2.1
3	D	186	VAL	2.1
3	D	24	GLY	2.1
1	A	231	SER	2.1
3	D	36	THR	2.1
3	D	47	GLU	2.1
1	B	160	ASP	2.1
3	D	1086	LEU	2.1
3	D	187	LYS	2.0
3	D	352	ASN	2.0
3	D	144	GLY	2.0
3	D	471	GLU	2.0
2	C	1096	ALA	2.0
2	C	105	THR	2.0
2	C	293	PHE	2.0
1	B	92	PRO	2.0
1	B	137	LYS	2.0
3	D	579	ASP	2.0
3	D	1111	ASP	2.0
1	A	189	ARG	2.0
3	D	37	LEU	2.0
3	D	205	TYR	2.0
2	C	319	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

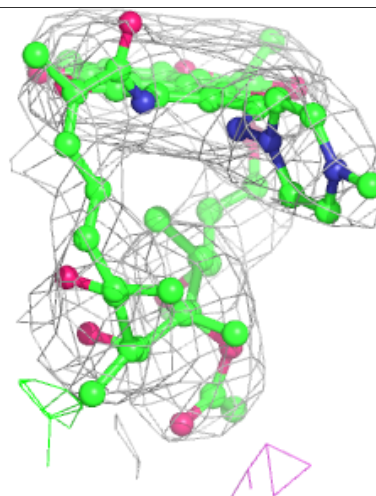
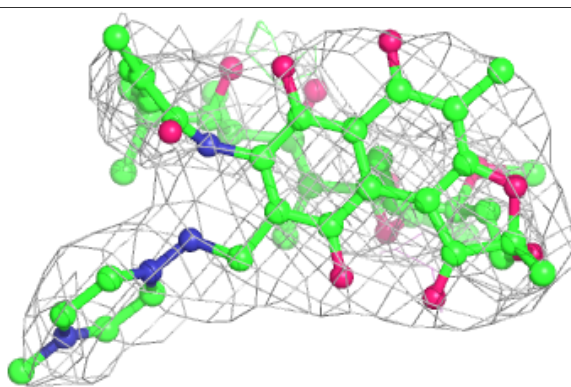
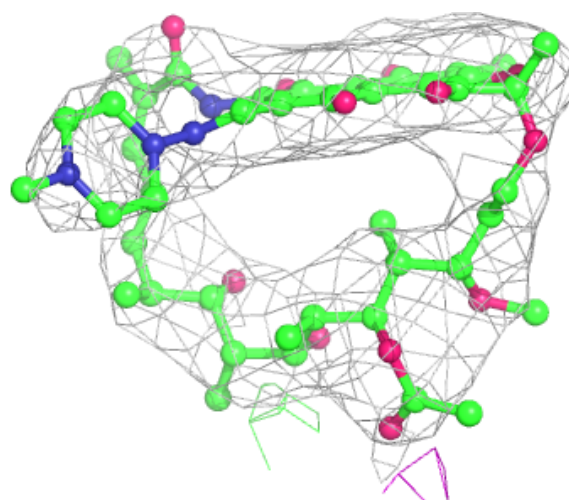
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	RFP	C	1120	59/59	0.92	0.26	44,47,60,63	0
6	ZN	D	1525	1/1	0.93	0.11	90,90,90,90	0
6	ZN	D	1526	1/1	0.96	0.18	52,52,52,52	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 RFP 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 ⓘ

There are no such residues in this entry.