



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:44 AM UTC

PDB ID : 6OW3 / pdb_00006ow3
Title : X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter variant -1T
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2019-05-09
Resolution : 2.77 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

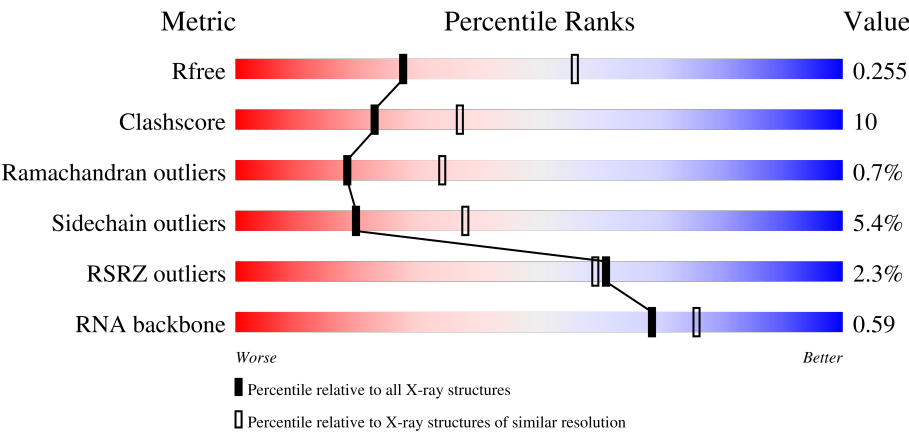
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



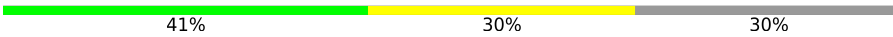
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)
RNA backbone	3983	1179 (3.00-2.52)

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

Mol	Chain	Length	Quality of chain
1	A	315	54%16%•28%
1	B	315	% 50%19%•29%
2	C	1119	2% 72%25%••
3	D	1524	% 72%23%••

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Mol	Chain	Length	Quality of chain
4	E	99	
5	F	423	
6	G	22	
7	H	27	
8	I	4	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28430 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8758	5542	1558	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total	C	N	O	S	0	0	0
			11722	7431	2065	2191	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*TP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			327	155	64	92	16			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*GP*AP*TP*CP*TP*GP*AP*TP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	19	Total	C	N	O	P	0	0	0
			392	188	73	113	18			

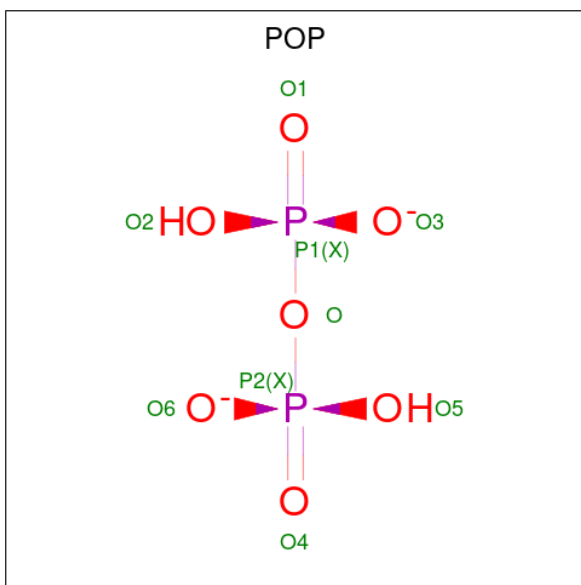
- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	4	Total	C	N	O	P	0	0	0
			101	40	20	35	6			

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	2	Total	Mg	0	0
			2	2		

- Molecule 10 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	O	P	0	0
			9	7	2		

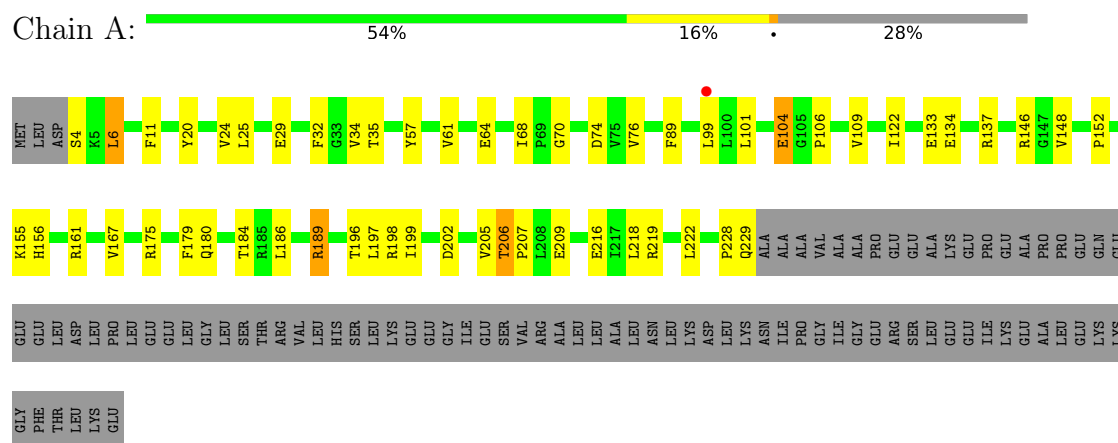
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

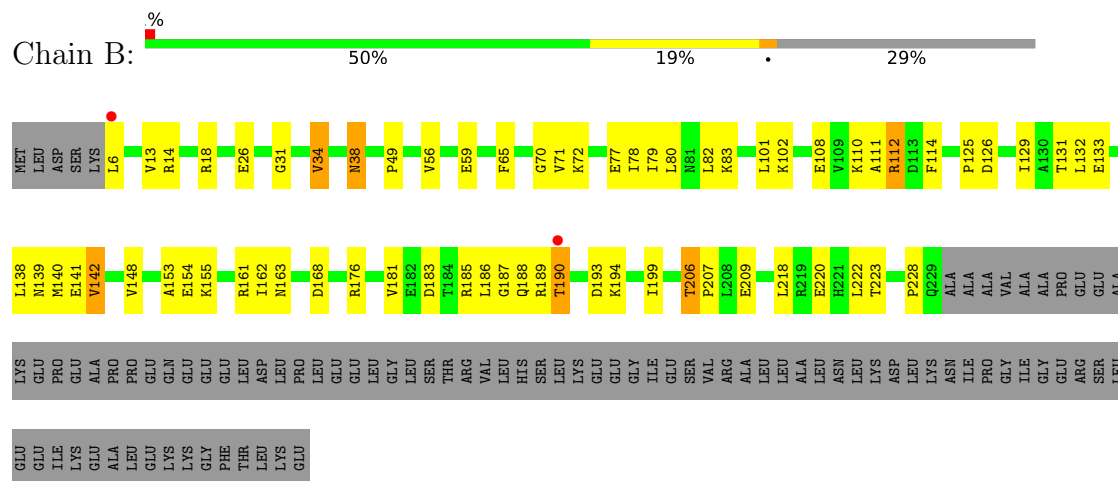
3 Residue-property plots

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

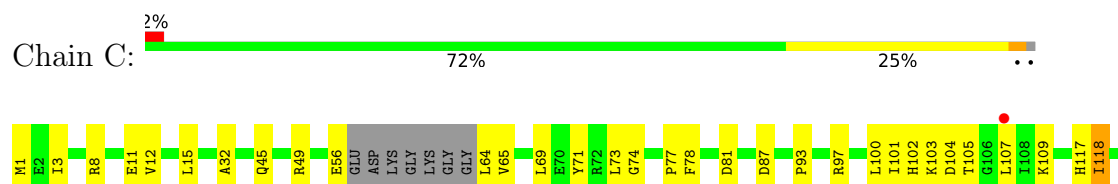
- Molecule 1: DNA-directed RNA polymerase subunit alpha

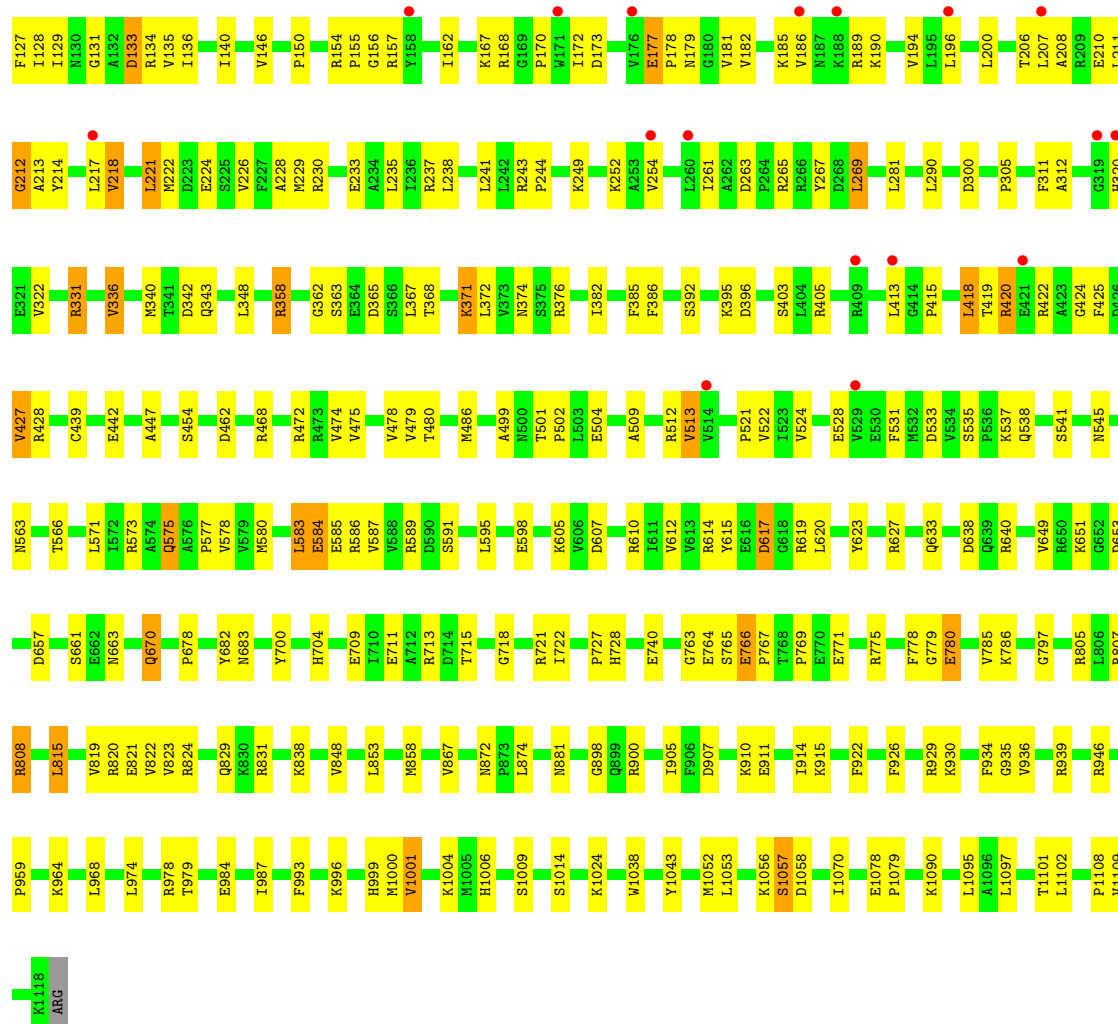


- Molecule 1: DNA-directed RNA polymerase subunit alpha

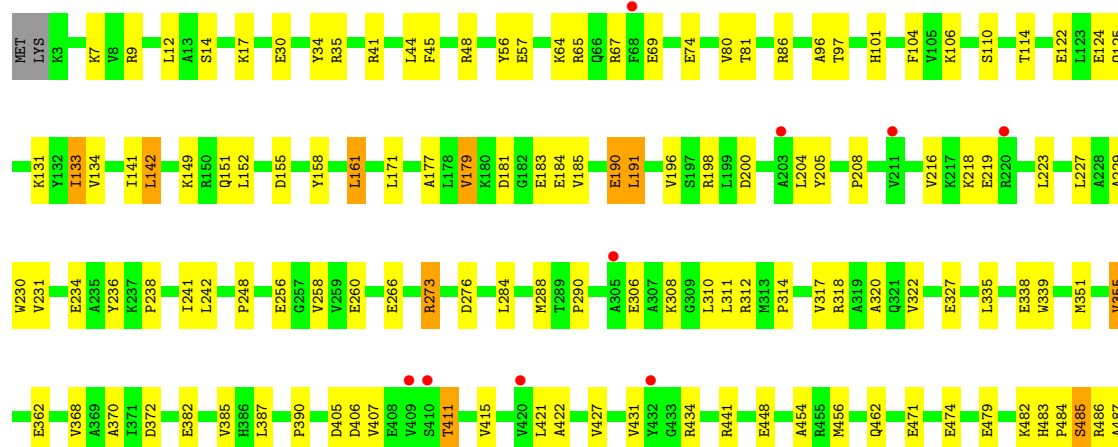
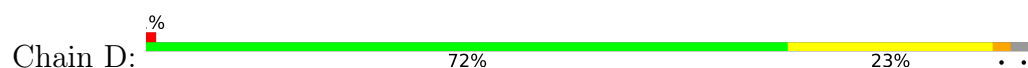


- Molecule 2: DNA-directed RNA polymerase subunit beta

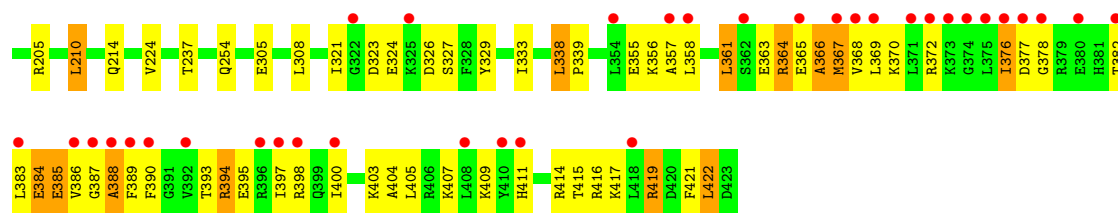




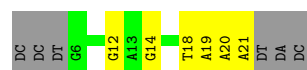
• Molecule 3: DNA-directed RNA polymerase subunit beta'



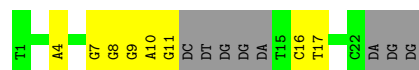




- Molecule 6: DNA (5'-D(P*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*TP*AP*AP*A)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*GP*AP*TP*CP*TP*GP*AP*TP*GP*C)-3')



- Molecule 8: RNA (5'-D(*(GTP))-R(P*GP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.19Å 101.83Å 295.75Å 90.00° 98.64° 90.00°	Depositor
Resolution (Å)	36.87 – 2.77 36.87 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.4 (36.87-2.77) 97.3 (36.87-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.217 , 0.255 0.217 , 0.255	Depositor DCC
R_{free} test set	2014 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.668	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28430	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0/1814	0.88	0/2466
1	B	0.47	0/1799	0.84	0/2447
2	C	0.48	0/8925	0.88	6/12073 (0.0%)
3	D	0.54	1/11928 (0.0%)	0.90	5/16127 (0.0%)
4	E	0.44	0/775	0.80	0/1045
5	F	0.49	0/2852	1.00	7/3837 (0.2%)
6	G	0.69	0/367	0.80	0/563
7	H	0.45	0/439	0.62	0/675
8	I	1.33	1/77 (1.3%)	1.02	0/119
All	All	0.51	2/28976 (0.0%)	0.89	18/39352 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
3	D	0	3
5	F	0	3
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	3	G	O3'-P	-7.80	1.49	1.61
3	D	704	ARG	C-N	-5.08	1.23	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	378	GLY	N-CA-C	-7.46	95.50	113.18
3	D	1300	SER	N-CA-C	6.98	120.04	109.23
3	D	739	ASP	N-CA-CB	6.92	121.33	110.87
5	F	388	ALA	N-CA-C	6.50	124.64	110.80
5	F	364	ARG	N-CA-C	6.46	118.40	111.36
3	D	1208	ASP	N-CA-C	-6.20	98.43	108.41
5	F	394	ARG	N-CA-C	6.18	123.97	110.80
5	F	419	ARG	CA-CB-CG	6.03	126.16	114.10
2	C	682	TYR	CA-C-N	5.79	132.85	122.38
2	C	682	TYR	C-N-CA	5.79	132.85	122.38
2	C	269	LEU	N-CA-C	-5.74	102.95	110.53
3	D	904	VAL	CB-CA-C	5.74	114.95	109.33
5	F	361	LEU	N-CA-C	-5.63	98.81	110.80
2	C	780	GLU	CA-C-N	5.46	128.62	120.87
2	C	780	GLU	C-N-CA	5.46	128.62	120.87
2	C	371	LYS	CA-CB-CG	5.32	124.75	114.10
3	D	740	PHE	CA-CB-CG	-5.15	108.65	113.80
5	F	422	LEU	CB-CG-CD2	5.01	125.73	110.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	766	GLU	Peptide
3	D	1195	GLN	Sidechain
3	D	583	ASP	Mainchain
3	D	903	ASP	Mainchain
5	F	363	GLU	Mainchain
5	F	366	ALA	Mainchain
5	F	389	PHE	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	1782	0	1834	40	0
1	B	1767	0	1816	42	0
2	C	8758	0	8852	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11722	0	11950	245	1
4	E	761	0	778	17	0
5	F	2807	0	2882	73	0
6	G	327	0	179	11	0
7	H	392	0	218	9	0
8	I	101	0	44	7	0
9	D	2	0	0	0	0
10	D	9	0	0	0	0
11	D	2	0	0	0	0
All	All	28430	0	28553	594	1

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 10.

All (594) 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)
5:F:382:THR:HG22	5:F:383:LEU:H	1.25	0.98
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.49	0.95
3:D:899:LEU:HD21	3:D:921:ARG:HD3	1.54	0.88
5:F:358:LEU:HB3	5:F:366:ALA:HB1	1.55	0.88
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.53	0.87
5:F:365:GLU:OE1	5:F:403:LYS:NZ	2.09	0.85
2:C:405:ARG:HD2	2:C:442:GLU:OE2	1.77	0.84
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.57	0.83
3:D:1294:VAL:O	3:D:1300:SER:OG	1.96	0.81
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.63	0.81
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.60	0.81
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.14	0.80
2:C:331:ARG:HH22	2:C:427:VAL:HG12	1.46	0.80
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.62	0.80
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.65	0.79
2:C:769:PRO:HD2	3:D:65:ARG:HH21	1.47	0.79
1:B:77:GLU:HG2	3:D:872:ARG:HH11	1.48	0.79
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.66	0.78
2:C:815:LEU:HD23	2:C:819:VAL:HG12	1.65	0.78
6:G:18:DT:H3	8:I:2:GTP:HN1	1.28	0.78
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.16	0.78
2:C:767:PRO:HB2	2:C:771:GLU:HG2	1.66	0.77
2:C:56:GLU:OE2	2:C:64:LEU:N	2.19	0.76
3:D:657:LEU:HG	3:D:661:MET:HE2	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.67	0.75
2:C:615:TYR:HH	2:C:623:TYR:HH	1.28	0.74
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.70	0.74
5:F:405:LEU:O	5:F:409:LYS:HG3	1.86	0.74
1:B:110:LYS:HB2	1:B:112:ARG:HH21	1.53	0.73
3:D:1254:GLN:HB2	3:D:1258:ARG:HB2	1.71	0.73
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.69	0.73
3:D:45:PHE:O	3:D:86:ARG:NH2	2.22	0.73
2:C:243:ARG:NH2	7:H:9:DG:O6	2.22	0.72
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.70	0.72
2:C:189:ARG:HH12	2:C:244:PRO:HD3	1.54	0.72
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.52	0.71
2:C:428:ARG:NH2	2:C:447:ALA:O	2.23	0.71
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.73	0.71
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.56	0.71
6:G:19:DA:C2	8:I:2:GTP:C2	2.80	0.70
3:D:669:ASN:HD22	5:F:417:LYS:HG2	1.55	0.70
1:A:175:ARG:HE	1:A:202:ASP:HB3	1.57	0.70
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.73	0.69
3:D:411:THR:HG22	5:F:178:ARG:HB3	1.73	0.69
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.75	0.68
2:C:154:ARG:HH22	2:C:178:PRO:HA	1.58	0.68
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.75	0.68
3:D:798:GLU:OE2	3:D:824:ASN:ND2	2.17	0.68
5:F:323:ASP:HB2	8:I:2:GTP:O3G	1.94	0.68
3:D:223:LEU:HD11	3:D:288:MET:HE1	1.75	0.68
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.76	0.68
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.75	0.67
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.76	0.67
3:D:800:LYS:NZ	3:D:819:GLY:O	2.28	0.67
3:D:1137:ARG:O	3:D:1141:GLU:HG3	1.95	0.67
1:B:78:ILE:HG21	1:B:140:MET:HE1	1.77	0.66
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.75	0.66
2:C:367:LEU:HA	2:C:371:LYS:HE2	1.78	0.66
5:F:382:THR:CG2	5:F:383:LEU:H	2.05	0.66
3:D:1314:LYS:H	3:D:1314:LYS:HD2	1.61	0.66
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.28	0.66
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.28	0.66
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.76	0.65
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.29	0.65
1:A:70:GLY:N	2:C:607:ASP:OD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1143:GLY:O	3:D:1147:ARG:HD2	1.96	0.64
3:D:1205:TYR:CZ	3:D:1366:LYS:HE3	2.32	0.64
3:D:1131:SER:OG	3:D:1132:LEU:N	2.31	0.64
2:C:853:LEU:HB2	2:C:858:MET:CE	2.27	0.64
5:F:383:LEU:HD22	5:F:394:ARG:HH22	1.62	0.64
2:C:764:GLU:C	2:C:766:GLU:H	2.03	0.64
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.30	0.64
3:D:1353:GLN:NE2	3:D:1365:ASP:OD1	2.23	0.64
2:C:211:LEU:O	2:C:213:ALA:N	2.23	0.63
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.79	0.63
3:D:122:GLU:HG2	3:D:152:LEU:HD11	1.80	0.63
5:F:364:ARG:HA	5:F:367:MET:HB2	1.81	0.63
2:C:207:LEU:HD13	2:C:221:LEU:HD11	1.80	0.62
3:D:702:LEU:HB3	3:D:745:MET:CE	2.29	0.62
5:F:400:ILE:O	5:F:404:ALA:N	2.28	0.62
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.81	0.62
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.34	0.62
5:F:400:ILE:HA	5:F:403:LYS:HB3	1.81	0.62
2:C:678:PRO:HA	2:C:683:ASN:HD22	1.64	0.62
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.82	0.62
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.27	0.62
6:G:19:DA:H2'	6:G:20:DA:C8	2.34	0.62
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.81	0.62
2:C:1078:GLU:HG2	2:C:1079:PRO:HD2	1.81	0.62
2:C:425:PHE:CD1	3:D:1079:LYS:HE3	2.35	0.62
2:C:996:LYS:HE2	2:C:1000:MET:HE2	1.82	0.62
1:B:65:PHE:CD2	3:D:809:PRO:HB2	2.34	0.61
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.82	0.61
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.16	0.61
2:C:649:VAL:HG13	2:C:653:ASP:HB2	1.81	0.61
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.82	0.61
1:B:77:GLU:HG2	3:D:872:ARG:NH1	2.15	0.61
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.15	0.61
2:C:715:THR:OG1	2:C:718:GLY:O	2.18	0.61
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.83	0.60
2:C:12:VAL:HG21	2:C:472:ARG:CD	2.31	0.60
5:F:414:ARG:HB3	5:F:414:ARG:HH11	1.66	0.60
3:D:573:MET:HE1	5:F:214:GLN:HG3	1.83	0.60
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.35	0.60
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.83	0.60
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1277:ILE:HG13	3:D:1278:ASP:H	1.66	0.60
2:C:214:TYR:HB3	2:C:217:LEU:HD12	1.85	0.59
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.85	0.59
2:C:911:GLU:OE2	3:D:1062:ARG:NH1	2.35	0.59
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.67	0.59
2:C:208:ALA:HB2	2:C:222:MET:HE1	1.85	0.58
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.85	0.58
3:D:133:ILE:HD12	3:D:152:LEU:HD23	1.84	0.58
1:B:56:VAL:HG23	1:B:142:VAL:HG12	1.86	0.58
2:C:229:MET:HE1	2:C:237:ARG:HH21	1.67	0.58
2:C:763:GLY:C	2:C:765:SER:H	2.11	0.58
5:F:368:VAL:HG13	5:F:390:PHE:CD2	2.38	0.58
3:D:485:SER:O	3:D:487:ALA:N	2.32	0.58
3:D:520:LEU:O	3:D:525:ARG:NH1	2.35	0.58
3:D:171:LEU:HD21	3:D:177:ALA:HB2	1.84	0.58
5:F:115:LYS:HD3	5:F:173:TYR:CE2	2.38	0.58
1:B:138:LEU:HD21	1:B:140:MET:HE3	1.84	0.58
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.67	0.58
3:D:179:VAL:HG11	3:D:191:LEU:HD12	1.86	0.57
2:C:627:ARG:HD2	2:C:638:ASP:OD1	2.04	0.57
2:C:807:ARG:HG2	2:C:821:GLU:HB3	1.86	0.57
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.87	0.57
3:D:97:THR:HG23	3:D:554:LEU:HD21	1.87	0.57
3:D:1281:VAL:CG2	3:D:1317:ASP:H	2.18	0.57
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.70	0.57
1:A:216:GLU:OE1	1:A:219:ARG:NH2	2.38	0.57
3:D:483:HIS:CE1	3:D:488:ARG:HD2	2.40	0.57
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.86	0.56
2:C:167:LYS:NZ	7:H:11:DG:H5"	2.20	0.56
2:C:775:ARG:HG3	2:C:780:GLU:O	2.06	0.56
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.41	0.56
5:F:382:THR:HG22	5:F:383:LEU:N	2.08	0.56
3:D:1386:ASP:OD2	3:D:1412:LYS:HD2	2.05	0.56
3:D:1499:ARG:NH1	4:E:84:ARG:HG2	2.20	0.56
5:F:122:LEU:HB2	5:F:127:ILE:HD11	1.88	0.56
3:D:67:ARG:HB3	5:F:377:ASP:OD1	2.04	0.56
1:A:6:LEU:HD23	1:A:29:GLU:OE2	2.06	0.56
2:C:214:TYR:O	2:C:218:VAL:HG23	2.06	0.56
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.88	0.56
5:F:368:VAL:HG13	5:F:390:PHE:HD2	1.70	0.56
2:C:420:ARG:HB2	2:C:420:ARG:NH2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.41	0.56
3:D:1290:LEU:HD23	3:D:1307:LYS:O	2.06	0.56
3:D:190:GLU:HG2	3:D:196:VAL:HG22	1.88	0.55
4:E:48:MET:HE2	4:E:50:THR:HG22	1.87	0.55
6:G:18:DT:H2'	6:G:19:DA:C8	2.41	0.55
6:G:20:DA:H8	6:G:20:DA:H5''	1.71	0.55
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.87	0.55
2:C:769:PRO:HD2	3:D:65:ARG:NH2	2.19	0.55
3:D:1047:LYS:HD2	3:D:1051:GLU:HG3	1.88	0.55
3:D:204:LEU:HD22	3:D:441:ARG:CZ	2.36	0.55
5:F:95:THR:HB	5:F:98:GLU:HG3	1.89	0.55
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.40	0.55
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.88	0.55
2:C:1:MET:HB2	2:C:898:GLY:O	2.07	0.55
1:B:101:LEU:HB2	1:B:114:PHE:CD2	2.42	0.55
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.89	0.55
2:C:358:ARG:HB3	2:C:372:LEU:HD12	1.89	0.54
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.06	0.54
3:D:1386:ASP:HB2	3:D:1412:LYS:HB3	1.89	0.54
2:C:607:ASP:HB3	2:C:610:ARG:H	1.72	0.54
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.90	0.54
3:D:208:PRO:HG3	3:D:387:LEU:HD22	1.89	0.54
3:D:573:MET:SD	5:F:210:LEU:HB3	2.48	0.54
3:D:1444:THR:O	3:D:1448:THR:HG23	2.07	0.54
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.87	0.54
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.90	0.54
3:D:1152:GLU:OE1	3:D:1161:GLU:HA	2.08	0.54
3:D:860:LEU:O	3:D:876:SER:HB2	2.07	0.54
2:C:331:ARG:NH2	2:C:427:VAL:HG12	2.18	0.54
2:C:1004:LYS:HD3	3:D:744:GLN:HE22	1.71	0.54
3:D:1198:TYR:CE2	3:D:1460:ILE:HD13	2.43	0.54
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.89	0.54
3:D:500:ARG:NH1	3:D:1390:LEU:HD21	2.23	0.53
3:D:658:LEU:HD23	3:D:661:MET:CE	2.38	0.53
3:D:1126:ASP:O	3:D:1130:ARG:HA	2.08	0.53
2:C:797:GLY:O	2:C:829:GLN:NE2	2.41	0.53
3:D:181:ASP:HB2	3:D:205:TYR:CG	2.43	0.53
3:D:702:LEU:HB3	3:D:745:MET:HE2	1.90	0.53
3:D:1084:THR:O	3:D:1088:THR:HG23	2.09	0.53
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.90	0.53
2:C:577:PRO:HG2	2:C:580:MET:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.43	0.53
3:D:351:MET:HE2	3:D:368:VAL:HG11	1.89	0.53
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.09	0.53
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.44	0.53
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.44	0.53
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.41	0.53
3:D:750:PRO:O	3:D:756:GLN:NE2	2.42	0.53
5:F:383:LEU:HD21	5:F:398:ARG:HH11	1.74	0.53
6:G:12:DG:H8	6:G:12:DG:C5'	2.22	0.53
3:D:895:VAL:HG11	3:D:922:LEU:HD21	1.90	0.53
5:F:172:ARG:O	5:F:176:ILE:HG12	2.09	0.53
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.90	0.52
5:F:419:ARG:O	5:F:422:LEU:HB2	2.09	0.52
2:C:425:PHE:CE2	3:D:1086:LEU:HD12	2.44	0.52
3:D:924:MET:HG2	4:E:7:ASP:OD1	2.09	0.52
2:C:102:HIS:CE1	2:C:104:ASP:HB2	2.44	0.52
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.90	0.52
3:D:1263:PHE:HA	3:D:1375:MET:HE1	1.92	0.52
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	1.91	0.52
2:C:999:HIS:HB3	2:C:1004:LYS:NZ	2.24	0.52
3:D:56:TYR:HE1	3:D:69:GLU:HG3	1.74	0.52
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.10	0.52
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.91	0.52
1:B:206:THR:HG22	1:B:209:GLU:H	1.75	0.52
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.38	0.52
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.45	0.52
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.42	0.52
2:C:211:LEU:HD23	2:C:311:PHE:HD2	1.74	0.51
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.92	0.51
2:C:595:LEU:HD21	2:C:623:TYR:HB3	1.93	0.51
2:C:263:ASP:C	2:C:265:ARG:H	2.18	0.51
2:C:367:LEU:HD23	2:C:371:LYS:HE2	1.91	0.51
2:C:598:GLU:O	2:C:651:LYS:HG3	2.10	0.51
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.93	0.51
3:D:973:GLN:HG2	3:D:974:ILE:HD13	1.91	0.51
2:C:587:VAL:O	2:C:591:SER:HB3	2.11	0.51
3:D:41:ARG:HH21	3:D:48:ARG:NH2	2.08	0.51
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.93	0.51
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.46	0.51
3:D:125:GLN:HB3	3:D:131:LYS:HB2	1.93	0.51
3:D:179:VAL:HB	3:D:183:GLU:OE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:HB3	1:A:137:ARG:HD3	1.93	0.50
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.10	0.50
2:C:154:ARG:O	2:C:156:GLY:N	2.44	0.50
2:C:229:MET:HB2	2:C:233:GLU:CB	2.39	0.50
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.46	0.50
2:C:424:GLY:O	2:C:427:VAL:HG23	2.11	0.50
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.94	0.50
2:C:168:ARG:NH2	2:C:265:ARG:O	2.45	0.50
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.94	0.50
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.47	0.50
5:F:115:LYS:HD3	5:F:173:TYR:HE2	1.75	0.50
1:A:206:THR:CG2	1:A:209:GLU:HG3	2.34	0.50
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.93	0.50
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.46	0.50
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.55	0.50
2:C:179:ASN:OD1	2:C:181:VAL:HG12	2.12	0.50
3:D:1305:LEU:HG	3:D:1309:ALA:HB3	1.93	0.50
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.94	0.49
3:D:1271:LYS:HG3	3:D:1272:ALA:O	2.12	0.49
3:D:1495:ILE:HG12	4:E:88:GLU:CG	2.36	0.49
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.41	0.49
3:D:241:ILE:HD13	3:D:310:LEU:HD22	1.93	0.49
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.94	0.49
2:C:12:VAL:HG21	2:C:472:ARG:NE	2.28	0.49
2:C:472:ARG:HD2	2:C:480:THR:O	2.13	0.49
2:C:573:ARG:HB2	2:C:670:GLN:NE2	2.28	0.49
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.95	0.49
1:A:104:GLU:HB3	1:A:137:ARG:CD	2.43	0.49
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.95	0.49
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.27	0.49
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.44	0.49
5:F:172:ARG:HG3	5:F:173:TYR:CD1	2.48	0.49
3:D:74:GLU:CD	3:D:74:GLU:H	2.21	0.49
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.48	0.49
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.46	0.49
5:F:91:VAL:O	5:F:193:ARG:NH2	2.38	0.49
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.78	0.49
1:A:32:PHE:HA	1:A:35:THR:HB	1.95	0.49
2:C:134:ARG:NH1	2:C:392:SER:O	2.46	0.49
2:C:563:ASN:O	2:C:566:THR:HB	2.12	0.49
2:C:420:ARG:HB2	2:C:420:ARG:CZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:425:PHE:HD1	3:D:1079:LYS:HE3	1.78	0.48
3:D:219:GLU:HB2	3:D:339:TRP:CH2	2.47	0.48
3:D:1283:ILE:HG12	3:D:1315:ASP:CG	2.38	0.48
2:C:224:GLU:CD	2:C:224:GLU:H	2.22	0.48
2:C:575:GLN:HG3	2:C:670:GLN:HA	1.95	0.48
2:C:858:MET:HG2	2:C:867:VAL:O	2.12	0.48
2:C:474:VAL:HG22	2:C:479:VAL:HG22	1.95	0.48
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.94	0.48
3:D:658:LEU:HA	3:D:661:MET:HE3	1.95	0.48
3:D:1291:SER:OG	3:D:1304:LYS:HG2	2.13	0.48
1:B:153:ALA:C	1:B:155:LYS:H	2.21	0.48
2:C:117:HIS:O	2:C:118:ILE:HD13	2.14	0.48
2:C:150:PRO:HG3	2:C:322:VAL:HG21	1.94	0.48
2:C:580:MET:HB3	2:C:584:GLU:CD	2.38	0.48
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.94	0.48
2:C:911:GLU:CD	3:D:1062:ARG:HH11	2.22	0.48
3:D:1108:ARG:HD2	3:D:1198:TYR:O	2.14	0.48
1:A:216:GLU:CD	1:A:219:ARG:HH22	2.22	0.48
2:C:212:GLY:H	2:C:218:VAL:HG11	1.78	0.48
2:C:226:VAL:O	2:C:229:MET:HG2	2.13	0.48
3:D:922:LEU:HB3	3:D:926:LYS:HD2	1.96	0.48
3:D:1093:TYR:OH	3:D:1441:GLN:OE1	2.28	0.48
2:C:331:ARG:HH22	2:C:427:VAL:CG1	2.21	0.48
2:C:713:ARG:CZ	2:C:715:THR:HG22	2.43	0.48
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.49	0.48
5:F:172:ARG:HG3	5:F:173:TYR:HD1	1.78	0.48
1:A:206:THR:HG22	1:A:209:GLU:CG	2.35	0.48
1:B:18:ARG:O	1:B:207:PRO:HD3	2.14	0.48
2:C:154:ARG:NH2	2:C:178:PRO:HA	2.25	0.48
3:D:1053:PHE:CE2	3:D:1072:ILE:HG23	2.48	0.48
2:C:605:LYS:HB2	2:C:612:VAL:HB	1.96	0.48
5:F:415:THR:C	5:F:417:LYS:H	2.21	0.48
1:B:70:GLY:O	1:B:133:GLU:HG3	2.14	0.47
2:C:229:MET:HE1	2:C:237:ARG:NH2	2.29	0.47
2:C:312:ALA:HB3	2:C:320:HIS:NE2	2.29	0.47
2:C:524:VAL:HG22	2:C:528:GLU:HB2	1.96	0.47
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.96	0.47
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.96	0.47
3:D:405:ASP:CG	3:D:406:ASP:H	2.23	0.47
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.96	0.47
3:D:883:ALA:HA	3:D:900:ILE:HD13	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1198:TYR:CZ	3:D:1460:ILE:HD13	2.49	0.47
3:D:1263:PHE:HD2	3:D:1375:MET:CE	2.27	0.47
5:F:366:ALA:O	5:F:370:LYS:HB2	2.14	0.47
2:C:374:ASN:OD1	2:C:376:ARG:HG2	2.14	0.47
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.49	0.47
5:F:127:ILE:O	5:F:131:VAL:HG23	2.15	0.47
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.97	0.47
2:C:709:GLU:HG3	2:C:824:ARG:HG2	1.97	0.47
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.96	0.47
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.97	0.47
3:D:986:ARG:HE	3:D:986:ARG:HA	1.78	0.47
5:F:368:VAL:HG11	5:F:400:ILE:HG13	1.95	0.47
1:B:161:ARG:HG3	1:B:162:ILE:O	2.15	0.47
2:C:605:LYS:HB3	2:C:610:ARG:NH1	2.30	0.47
3:D:131:LYS:N	3:D:456:MET:HE2	2.30	0.47
3:D:258:VAL:HG12	3:D:273:ARG:O	2.15	0.47
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.96	0.47
5:F:193:ARG:HB3	7:H:7:DG:H5''	1.97	0.47
5:F:414:ARG:HB3	5:F:414:ARG:NH1	2.29	0.47
2:C:243:ARG:NH1	7:H:10:DA:N1	2.62	0.47
2:C:911:GLU:O	2:C:915:LYS:HG2	2.14	0.47
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.63	0.47
2:C:420:ARG:NE	8:I:2:GTP:O1B	2.48	0.47
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.97	0.47
5:F:394:ARG:HG3	5:F:395:GLU:N	2.29	0.47
5:F:415:THR:O	5:F:417:LYS:N	2.44	0.46
2:C:189:ARG:HH12	2:C:244:PRO:CD	2.26	0.46
6:G:19:DA:C2	8:I:2:GTP:N1	2.82	0.46
1:B:101:LEU:HB2	1:B:114:PHE:CE2	2.50	0.46
3:D:134:VAL:HG23	3:D:149:LYS:HA	1.97	0.46
3:D:1087:ARG:HG3	3:D:1256:LEU:HD23	1.98	0.46
3:D:134:VAL:CG2	3:D:151:GLN:H	2.28	0.46
3:D:638:LYS:HA	3:D:638:LYS:HD3	1.74	0.46
3:D:671:LYS:HE3	5:F:421:PHE:HA	1.97	0.46
3:D:1236:LEU:HG	3:D:1359:GLN:HG3	1.98	0.46
2:C:249:LYS:HB3	2:C:252:LYS:HB2	1.97	0.46
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.49	0.46
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.49	0.46
2:C:763:GLY:C	2:C:765:SER:N	2.72	0.46
3:D:216:VAL:HB	3:D:382:GLU:HG2	1.97	0.46
6:G:19:DA:H4'	6:G:20:DA:OP1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:O	1:A:155:LYS:HB2	2.16	0.46
1:B:31:GLY:N	1:B:193:ASP:OD1	2.44	0.46
2:C:206:THR:O	2:C:210:GLU:HB2	2.16	0.46
2:C:722:ILE:HD12	2:C:821:GLU:HG3	1.98	0.46
3:D:630:VAL:HA	3:D:744:GLN:HG2	1.98	0.46
2:C:617:ASP:OD1	2:C:617:ASP:N	2.48	0.45
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.23	0.45
1:A:20:TYR:C	1:A:207:PRO:HG2	2.41	0.45
2:C:77:PRO:HB2	2:C:78:PHE:CD1	2.51	0.45
2:C:778:PHE:C	2:C:780:GLU:H	2.24	0.45
5:F:355:GLU:C	5:F:357:ALA:H	2.23	0.45
5:F:368:VAL:CG1	5:F:397:ILE:HD12	2.46	0.45
1:A:198:ARG:O	1:A:199:ILE:HD13	2.16	0.45
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.99	0.45
3:D:56:TYR:CE1	3:D:69:GLU:HG3	2.51	0.45
6:G:20:DA:H2''	6:G:21:DA:OP1	2.15	0.45
1:B:188:GLN:NE2	1:B:189:ARG:HG3	2.31	0.45
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.16	0.45
5:F:82:ARG:HB2	7:H:8:DG:O6	2.16	0.45
5:F:329:TYR:CE2	5:F:333:ILE:HD11	2.51	0.45
2:C:185:LYS:HE2	2:C:190:LYS:HE3	1.97	0.45
2:C:974:LEU:HD12	2:C:974:LEU:HA	1.64	0.45
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.97	0.45
3:D:632:VAL:O	3:D:727:GLN:HA	2.16	0.45
3:D:1217:ILE:HD12	3:D:1480:PHE:CZ	2.51	0.45
3:D:741:ASP:OD1	3:D:743:ASP:OD1	2.35	0.45
3:D:1154:GLU:OE2	3:D:1159:ARG:HB2	2.16	0.45
5:F:368:VAL:HG13	5:F:397:ILE:HD12	1.98	0.45
5:F:407:LYS:O	5:F:411:HIS:HD2	2.00	0.45
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.78	0.45
3:D:284:LEU:CD1	3:D:290:PRO:HG3	2.47	0.45
8:I:2:GTP:O1A	8:I:2:GTP:C8	2.70	0.45
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.99	0.45
3:D:1092:GLY:HA3	6:G:14:DG:O4'	2.17	0.45
3:D:1290:LEU:HB3	3:D:1305:LEU:HD23	1.99	0.45
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.98	0.44
2:C:177:GLU:HG3	2:C:178:PRO:HD2	2.00	0.44
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.98	0.44
3:D:1277:ILE:HG13	3:D:1278:ASP:N	2.31	0.44
1:B:185:ARG:NH1	1:B:187:GLY:O	2.50	0.44
2:C:764:GLU:C	2:C:766:GLU:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.98	0.44
1:A:101:LEU:HD11	1:A:109:VAL:CG1	2.47	0.44
1:B:59:GLU:OE1	1:B:139:ASN:ND2	2.51	0.44
2:C:721:ARG:HH22	2:C:785:VAL:HG11	1.82	0.44
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.99	0.44
5:F:94:LEU:HD13	5:F:99:GLU:HA	1.99	0.44
2:C:340:MET:HE2	2:C:382:ILE:HD12	2.00	0.44
2:C:815:LEU:HD23	2:C:819:VAL:CG1	2.41	0.44
3:D:322:VAL:HG22	3:D:335:LEU:HD23	1.99	0.44
3:D:411:THR:O	5:F:178:ARG:NH1	2.43	0.44
5:F:369:LEU:HD22	5:F:404:ALA:HB1	1.99	0.44
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.99	0.44
2:C:229:MET:HE2	2:C:229:MET:HB3	1.80	0.44
2:C:1097:LEU:HA	2:C:1097:LEU:HD23	1.66	0.44
3:D:171:LEU:HD22	3:D:390:PRO:HG2	2.00	0.44
5:F:237:THR:OG1	7:H:4:DA:H8	2.01	0.44
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.77	0.44
4:E:36:LYS:CG	4:E:93:TYR:HB3	2.47	0.44
5:F:384:GLU:CD	5:F:384:GLU:H	2.26	0.44
5:F:393:THR:HG22	5:F:394:ARG:N	2.31	0.44
2:C:135:VAL:HG23	2:C:395:LYS:HG3	2.00	0.44
2:C:418:LEU:H	2:C:418:LEU:HD12	1.82	0.44
3:D:869:MET:HE2	3:D:869:MET:HB3	1.78	0.44
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.53	0.44
8:I:2:GTP:O5'	8:I:2:GTP:H8	2.01	0.44
3:D:669:ASN:HB3	5:F:417:LYS:HE2	2.00	0.43
3:D:907:GLU:OE2	3:D:909:ASN:N	2.44	0.43
5:F:361:LEU:HD21	5:F:411:HIS:CG	2.53	0.43
1:B:71:VAL:HG22	1:B:132:LEU:HG	2.00	0.43
3:D:185:VAL:O	3:D:200:ASP:HA	2.17	0.43
3:D:238:PRO:CD	3:D:318:ARG:HG3	2.41	0.43
4:E:14:ASP:OD1	4:E:18:ARG:NH1	2.51	0.43
1:A:228:PRO:HB3	1:B:13:VAL:HG21	2.00	0.43
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.99	0.43
2:C:778:PHE:O	2:C:780:GLU:N	2.52	0.43
2:C:946:ARG:NH1	2:C:984:GLU:OE2	2.51	0.43
3:D:351:MET:HG2	3:D:370:ALA:HB2	2.00	0.43
1:B:185:ARG:HB3	1:B:190:THR:HG23	2.00	0.43
2:C:127:PHE:HB3	2:C:129:ILE:HD13	2.00	0.43
2:C:211:LEU:HD22	2:C:218:VAL:HG13	2.00	0.43
2:C:910:LYS:O	2:C:914:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.00	0.43
3:D:1089:ALA:HA	6:G:14:DG:C8	2.54	0.43
1:A:106:PRO:CG	1:A:134:GLU:HG2	2.46	0.43
2:C:56:GLU:HG3	2:C:64:LEU:O	2.19	0.43
2:C:154:ARG:C	2:C:156:GLY:H	2.26	0.43
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.83	0.43
3:D:134:VAL:HG22	3:D:151:GLN:H	1.82	0.43
3:D:322:VAL:HG22	3:D:335:LEU:CD2	2.49	0.43
3:D:501:ALA:HB1	3:D:1452:ILE:HG22	2.01	0.43
3:D:972:LEU:HD13	3:D:972:LEU:HA	1.61	0.43
3:D:1402:ALA:O	3:D:1406:ARG:HG3	2.18	0.43
1:A:4:SER:HB3	1:A:189:ARG:HH21	1.82	0.43
3:D:431:VAL:HG21	3:D:448:GLU:HG2	1.99	0.43
3:D:806:PHE:O	3:D:829:VAL:HA	2.18	0.43
5:F:361:LEU:HD13	5:F:407:LYS:HB3	2.01	0.43
5:F:394:ARG:NH1	5:F:395:GLU:OE2	2.48	0.43
1:A:11:PHE:O	1:B:228:PRO:HA	2.18	0.43
1:A:156:HIS:NE2	1:A:167:VAL:O	2.41	0.43
1:A:218:LEU:HG	1:B:222:LEU:HD11	2.00	0.43
1:A:206:THR:HG22	1:A:209:GLU:H	1.82	0.43
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.52	0.43
1:B:34:VAL:HG12	1:B:181:VAL:HG21	2.00	0.43
1:B:80:LEU:HD22	3:D:844:ALA:HA	2.01	0.43
2:C:468:ARG:HA	2:C:486:MET:O	2.18	0.43
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.99	0.43
3:D:711:LEU:HD13	3:D:778:LEU:HD13	2.01	0.43
3:D:838:ARG:HD3	3:D:874:GLU:CD	2.44	0.43
5:F:148:LYS:HE3	5:F:148:LYS:HB2	1.74	0.43
2:C:3:ILE:HD13	2:C:900:ARG:HB2	2.01	0.43
2:C:589:ARG:HE	2:C:589:ARG:HB2	1.69	0.43
2:C:614:ARG:HE	2:C:620:LEU:HD13	1.84	0.43
1:B:38:ASN:OD1	2:C:979:THR:HG22	2.19	0.42
2:C:405:ARG:O	2:C:405:ARG:HG2	2.17	0.42
3:D:1122:LEU:HD13	3:D:1178:ALA:HB2	2.01	0.42
3:D:1299:PHE:HD1	3:D:1299:PHE:HA	1.70	0.42
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.19	0.42
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.20	0.42
5:F:385:GLU:C	5:F:387:GLY:H	2.27	0.42
1:A:180:GLN:NE2	2:C:935:GLY:O	2.51	0.42
2:C:167:LYS:HZ1	7:H:11:DG:H5"	1.83	0.42
3:D:17:LYS:HB2	3:D:17:LYS:HE2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:ARG:HB2	5:F:377:ASP:O	2.19	0.42
3:D:479:GLU:OE1	3:D:482:LYS:NZ	2.52	0.42
3:D:526:PRO:HB2	3:D:528:VAL:HG13	2.00	0.42
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.00	0.42
1:B:220:GLU:O	1:B:223:THR:OG1	2.31	0.42
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.38	0.42
3:D:882:PHE:HE1	3:D:900:ILE:HG23	1.84	0.42
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.55	0.42
5:F:81:VAL:HG22	5:F:210:LEU:CD1	2.49	0.42
5:F:358:LEU:O	5:F:366:ALA:HB2	2.20	0.42
1:B:110:LYS:C	1:B:129:ILE:HD12	2.44	0.42
2:C:69:LEU:HB2	2:C:97:ARG:O	2.19	0.42
2:C:269:LEU:HD12	2:C:269:LEU:HA	1.79	0.42
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	2.01	0.42
3:D:317:VAL:HG23	3:D:339:TRP:HB3	2.02	0.42
4:E:36:LYS:HG3	4:E:93:TYR:HB3	2.00	0.42
5:F:395:GLU:OE1	5:F:398:ARG:HD3	2.18	0.42
2:C:167:LYS:HZ3	7:H:11:DG:H5"	1.85	0.42
2:C:185:LYS:HE2	2:C:185:LYS:HB2	1.96	0.42
2:C:281:LEU:HD13	2:C:305:PRO:HB2	2.02	0.42
3:D:1438:ALA:N	3:D:1446:VAL:HG11	2.34	0.42
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.34	0.42
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.19	0.42
3:D:693:GLU:HB3	4:E:48:MET:HE1	2.02	0.42
3:D:1355:VAL:O	3:D:1359:GLN:HG2	2.20	0.42
3:D:1380:GLU:HB2	3:D:1420:LEU:HD22	2.00	0.42
1:A:61:VAL:HG21	1:A:68:ILE:HD11	2.02	0.42
2:C:154:ARG:HH12	2:C:178:PRO:HB3	1.84	0.42
2:C:439:CYS:HB2	2:C:541:SER:HB3	2.02	0.42
2:C:905:ILE:C	2:C:907:ASP:H	2.28	0.42
2:C:1009:SER:HB3	3:D:651:GLU:O	2.19	0.42
3:D:1420:LEU:HD12	3:D:1420:LEU:HA	1.91	0.42
2:C:140:ILE:HD13	2:C:331:ARG:HH11	1.84	0.42
2:C:999:HIS:HB3	2:C:1004:LYS:HZ2	1.84	0.42
3:D:618:LEU:HD13	3:D:618:LEU:HA	1.89	0.42
1:A:25:LEU:HD12	1:A:25:LEU:HA	1.86	0.41
2:C:56:GLU:HG2	2:C:64:LEU:HB2	2.02	0.41
2:C:200:LEU:HD13	2:C:300:ASP:HB2	2.00	0.41
2:C:926:PHE:CZ	2:C:930:LYS:HD3	2.55	0.41
3:D:1112:CYS:SG	3:D:1114:THR:HG22	2.60	0.41
5:F:166:LEU:HD23	5:F:166:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.35	0.41
1:A:101:LEU:HD21	1:A:109:VAL:HG11	2.02	0.41
2:C:207:LEU:CD1	2:C:221:LEU:HD11	2.50	0.41
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.52	0.41
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.85	0.41
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.55	0.41
4:E:12:MET:HE1	4:E:68:LEU:O	2.20	0.41
2:C:65:VAL:N	2:C:101:ILE:O	2.45	0.41
2:C:763:GLY:O	2:C:766:GLU:HG2	2.19	0.41
2:C:881:ASN:OD1	2:C:881:ASN:N	2.53	0.41
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.21	0.41
3:D:689:ASP:CG	4:E:51:LEU:HD11	2.45	0.41
3:D:763:MET:HE2	3:D:763:MET:HB3	1.78	0.41
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.55	0.41
1:B:132:LEU:HD21	1:B:138:LEU:HB2	2.02	0.41
3:D:703:ASN:HA	3:D:712:GLY:O	2.20	0.41
3:D:924:MET:HB3	3:D:924:MET:HE2	1.60	0.41
1:A:216:GLU:CD	1:A:219:ARG:NH2	2.78	0.41
1:B:72:LYS:HB3	1:B:131:THR:OG1	2.19	0.41
1:B:79:ILE:HA	1:B:82:LEU:HD12	2.02	0.41
2:C:127:PHE:O	2:C:133:ASP:HA	2.20	0.41
1:A:206:THR:CG2	1:A:209:GLU:H	2.33	0.41
2:C:420:ARG:C	2:C:422:ARG:H	2.27	0.41
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	2.02	0.41
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.20	0.41
4:E:37:ASN:HB3	4:E:93:TYR:CG	2.56	0.41
2:C:170:PRO:HD2	2:C:267:TYR:CE2	2.56	0.41
2:C:1001:VAL:HG13	3:D:630:VAL:HB	2.03	0.41
3:D:65:ARG:HH11	5:F:376:ILE:HA	1.86	0.41
3:D:288:MET:HA	3:D:306:GLU:O	2.20	0.41
3:D:1014:ASN:OD1	3:D:1014:ASN:N	2.53	0.41
3:D:1149:LEU:HG	3:D:1166:LEU:HD21	2.01	0.41
2:C:102:HIS:HB3	2:C:105:THR:HB	2.02	0.41
2:C:263:ASP:O	2:C:265:ARG:N	2.51	0.41
2:C:486:MET:HE1	2:C:531:PHE:CE2	2.55	0.41
3:D:1478:SER:O	3:D:1482:ARG:HB2	2.20	0.41
1:B:112:ARG:HG3	1:B:125:PRO:O	2.20	0.41
1:B:162:ILE:O	1:B:163:ASN:HB2	2.21	0.41
2:C:133:ASP:HB3	2:C:395:LYS:HD2	2.02	0.41
2:C:211:LEU:HD23	2:C:311:PHE:CD2	2.53	0.41
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:65:ARG:NH1	5:F:376:ILE:HA	2.36	0.41
3:D:527:MET:HE2	3:D:527:MET:HB2	1.88	0.41
2:C:512:ARG:HG3	2:C:512:ARG:O	2.20	0.41
3:D:219:GLU:HB2	3:D:339:TRP:HH2	1.84	0.41
3:D:227:LEU:C	3:D:229:ALA:H	2.29	0.41
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.21	0.41
5:F:386:VAL:HG13	5:F:390:PHE:CE1	2.55	0.41
2:C:128:ILE:C	2:C:129:ILE:HD12	2.46	0.40
2:C:419:THR:HG22	2:C:420:ARG:H	1.86	0.40
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	2.03	0.40
4:E:37:ASN:HB3	4:E:93:TYR:CD1	2.56	0.40
7:H:16:DC:H4'	7:H:17:DT:OP1	2.21	0.40
1:A:74:ASP:OD1	1:A:76:VAL:HB	2.21	0.40
1:A:99:LEU:HD21	1:A:122:ILE:HD11	2.03	0.40
2:C:32:ALA:HB2	2:C:73:LEU:HD12	2.04	0.40
2:C:238:LEU:O	2:C:241:LEU:HB2	2.22	0.40
2:C:1053:LEU:HA	3:D:621:LYS:HD2	2.03	0.40
5:F:321:ILE:HD12	5:F:321:ILE:HG23	1.91	0.40
2:C:501:THR:HG21	2:C:513:VAL:HB	2.03	0.40
2:C:1056:LYS:HG2	3:D:625:TYR:HD2	1.86	0.40
2:C:475:VAL:O	2:C:478:VAL:HG12	2.22	0.40
2:C:535:SER:O	2:C:538:GLN:HG2	2.22	0.40
2:C:657:ASP:OD2	2:C:663:ASN:N	2.50	0.40
2:C:911:GLU:CD	3:D:1062:ARG:NH1	2.80	0.40
3:D:284:LEU:HD22	3:D:288:MET:HE2	2.04	0.40
3:D:387:LEU:HD23	3:D:387:LEU:HA	1.94	0.40
3:D:407:VAL:HG23	3:D:422:ALA:HB2	2.04	0.40
4:E:30:LEU:HB3	4:E:35:PHE:CE1	2.57	0.40
5:F:308:LEU:HD23	5:F:308:LEU:HA	1.91	0.40
2:C:348:LEU:HA	2:C:348:LEU:HD12	1.86	0.40
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.87	0.40
2:C:501:THR:HA	2:C:502:PRO:HD3	1.98	0.40
2:C:598:GLU:N	2:C:615:TYR:OH	2.50	0.40
2:C:633:GLN:OE1	2:C:633:GLN:N	2.54	0.40
2:C:838:LYS:HE3	3:D:741:ASP:O	2.22	0.40
3:D:110:SER:O	3:D:114:THR:HG23	2.20	0.40
3:D:977:ALA:HB1	3:D:982:PHE:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_1359]	2.08	0.12

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	224/315 (71%)	220 (98%)	4 (2%)	0	100	100
1	B	222/315 (70%)	210 (95%)	11 (5%)	1 (0%)	24	43
2	C	1107/1119 (99%)	1062 (96%)	36 (3%)	9 (1%)	16	30
3	D	1480/1524 (97%)	1434 (97%)	39 (3%)	7 (0%)	24	43
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	11	22
5	F	344/423 (81%)	319 (93%)	18 (5%)	7 (2%)	6	11
All	All	3469/3795 (91%)	3334 (96%)	110 (3%)	25 (1%)	18	34

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	212	GLY
2	C	363	SER
3	D	486	ARG
5	F	324	GLU
5	F	388	ALA
2	C	228	ALA
2	C	362	GLY
2	C	365	ASP
3	D	484	PRO
5	F	327	SER
5	F	384	GLU
5	F	385	GLU
5	F	416	ARG
2	C	779	GLY
3	D	485	SER

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Mol	Chain	Res	Type
5	F	356	LYS
1	B	154	GLU
2	C	155	PRO
2	C	418	LEU
3	D	1050	GLY
3	D	320	ALA
4	E	94	PRO
3	D	1049	SER
3	D	831	GLY
2	C	415	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/273 (73%)	188 (94%)	11 (6%)	19	37
1	B	197/273 (72%)	185 (94%)	12 (6%)	17	31
2	C	934/941 (99%)	887 (95%)	47 (5%)	22	42
3	D	1250/1279 (98%)	1172 (94%)	78 (6%)	16	31
4	E	83/88 (94%)	83 (100%)	0	100	100
5	F	301/371 (81%)	290 (96%)	11 (4%)	30	54
All	All	2964/3225 (92%)	2805 (95%)	159 (5%)	20	38

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	104	GLU
1	A	133	GLU
1	A	148	VAL
1	A	184	THR
1	A	186	LEU
1	A	189	ARG

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Mol	Chain	Res	Type
1	A	205	VAL
1	A	206	THR
1	A	229	GLN
1	B	6	LEU
1	B	14	ARG
1	B	34	VAL
1	B	38	ASN
1	B	112	ARG
1	B	126	ASP
1	B	142	VAL
1	B	183	ASP
1	B	186	LEU
1	B	190	THR
1	B	199	ILE
1	B	206	THR
2	C	8	ARG
2	C	15	LEU
2	C	49	ARG
2	C	81	ASP
2	C	103	LYS
2	C	107	LEU
2	C	118	ILE
2	C	133	ASP
2	C	177	GLU
2	C	182	VAL
2	C	194	VAL
2	C	196	LEU
2	C	218	VAL
2	C	221	LEU
2	C	230	ARG
2	C	261	ILE
2	C	331	ARG
2	C	336	VAL
2	C	342	ASP
2	C	358	ARG
2	C	413	LEU
2	C	420	ARG
2	C	427	VAL
2	C	454	SER
2	C	513	VAL
2	C	522	VAL
2	C	575	GLN

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Mol	Chain	Res	Type
2	C	578	VAL
2	C	583	LEU
2	C	584	GLU
2	C	585	GLU
2	C	586	ARG
2	C	617	ASP
2	C	640	ARG
2	C	661	SER
2	C	670	GLN
2	C	786	LYS
2	C	808	ARG
2	C	815	LEU
2	C	820	ARG
2	C	848	VAL
2	C	939	ARG
2	C	968	LEU
2	C	978	ARG
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
3	D	30	GLU
3	D	80	VAL
3	D	81	THR
3	D	106	LYS
3	D	133	ILE
3	D	141	ILE
3	D	142	LEU
3	D	155	ASP
3	D	161	LEU
3	D	179	VAL
3	D	184	GLU
3	D	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	230	TRP
3	D	231	VAL
3	D	234	GLU
3	D	256	GLU
3	D	273	ARG
3	D	276	ASP
3	D	312	ARG
3	D	355	VAL

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Mol	Chain	Res	Type
3	D	362	GLU
3	D	372	ASP
3	D	411	THR
3	D	415	VAL
3	D	421	LEU
3	D	427	VAL
3	D	434	ARG
3	D	471	GLU
3	D	525	ARG
3	D	548	ILE
3	D	572	ARG
3	D	587	ARG
3	D	618	LEU
3	D	632	VAL
3	D	650	LEU
3	D	709	HIS
3	D	739	ASP
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	810	GLU
3	D	813	LEU
3	D	817	GLU
3	D	864	VAL
3	D	875	THR
3	D	894	LYS
3	D	904	VAL
3	D	972	LEU
3	D	973	GLN
3	D	995	LEU
3	D	997	THR
3	D	1014	ASN
3	D	1039	CYS
3	D	1041	LEU
3	D	1062	ARG
3	D	1154	GLU
3	D	1155	VAL
3	D	1188	VAL
3	D	1195	GLN
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL

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Mol	Chain	Res	Type
3	D	1236	LEU
3	D	1271	LYS
3	D	1284	GLU
3	D	1290	LEU
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP
3	D	1408	ILE
3	D	1418	LYS
3	D	1422	MET
3	D	1455	LYS
3	D	1470	ARG
3	D	1486	VAL
3	D	1493	LYS
5	F	98	GLU
5	F	125	ASP
5	F	159	ILE
5	F	205	ARG
5	F	210	LEU
5	F	254	GLN
5	F	326	ASP
5	F	338	LEU
5	F	367	MET
5	F	372	ARG
5	F	376	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	B	63	HIS
1	B	212	ASN
2	C	91	GLN
2	C	102	HIS
2	C	448	ASN
2	C	556	ASN
2	C	683	ASN
2	C	728	HIS
2	C	834	GLN
2	C	991	GLN
3	D	388	HIS
3	D	714	GLN

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Mol	Chain	Res	Type
3	D	724	GLN
3	D	737	ASN
3	D	744	GLN
3	D	1025	GLN
3	D	1195	GLN
3	D	1359	GLN
4	E	49	GLN
5	F	83	GLN
5	F	217	ASN
5	F	248	ASN
5	F	254	GLN
5	F	411	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	3/4 (75%)	0	1 (33%)

There are no RNA backbone outliers to report.

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	2	GTP

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 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	$\# Z > 2$
10	POP	D	1602	-	6,8,8	0.90	0	12,13,13	0.71	0

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
10	POP	D	1602	-	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	226/315 (71%)	0.11	1 (0%) 88 89	65, 88, 111, 123	0
1	B	224/315 (71%)	0.13	2 (0%) 81 81	63, 90, 120, 134	0
2	C	1111/1119 (99%)	0.15	18 (1%) 70 69	50, 87, 154, 180	0
3	D	1484/1524 (97%)	0.03	20 (1%) 75 75	45, 81, 145, 175	0
4	E	94/99 (94%)	0.54	3 (3%) 50 48	60, 98, 137, 147	0
5	F	346/423 (81%)	0.42	36 (10%) 11 11	56, 97, 180, 196	0
6	G	16/22 (72%)	-0.14	0 100 100	56, 92, 179, 180	0
7	H	19/27 (70%)	0.10	0 100 100	82, 125, 162, 166	0
8	I	3/4 (75%)	-0.76	0 100 100	58, 58, 64, 73	0
All	All	3523/3848 (91%)	0.13	80 (2%) 61 59	45, 87, 154, 196	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	369	LEU	5.1
5	F	400	ILE	4.5
5	F	375	LEU	4.2
3	D	409	VAL	4.0
5	F	376	ILE	3.7
5	F	373	LYS	3.6
4	E	32	ARG	3.6
5	F	374	GLY	3.6
5	F	397	ILE	3.4
5	F	325	LYS	3.4
5	F	372	ARG	3.4
2	C	171	TRP	3.3
3	D	1502	ALA	3.3
2	C	107	LEU	3.3
2	C	176	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
5	F	386	VAL	3.1
5	F	358	LEU	3.0
3	D	68	PHE	3.0
3	D	1283	ILE	3.0
1	B	190	THR	2.9
3	D	1128	VAL	2.9
3	D	1490	LYS	2.9
5	F	367	MET	2.9
2	C	186	VAL	2.9
5	F	408	LEU	2.9
3	D	211	VAL	2.8
2	C	207	LEU	2.8
5	F	390	PHE	2.8
3	D	203	ALA	2.8
5	F	378	GLY	2.7
2	C	254	VAL	2.7
5	F	392	VAL	2.7
3	D	1498	ALA	2.7
5	F	377	ASP	2.7
1	A	99	LEU	2.5
5	F	383	LEU	2.5
5	F	357	ALA	2.5
3	D	1234	THR	2.5
2	C	514	VAL	2.5
5	F	368	VAL	2.5
5	F	389	PHE	2.5
4	E	85	LEU	2.4
5	F	418	LEU	2.4
2	C	421	GLU	2.4
2	C	188	LYS	2.4
3	D	1494	ALA	2.4
1	B	6	LEU	2.3
2	C	260	LEU	2.3
2	C	413	LEU	2.3
5	F	396	ARG	2.3
3	D	420	VAL	2.3
5	F	78	SER	2.3
4	E	94	PRO	2.3
2	C	217	LEU	2.3
5	F	354	LEU	2.3
5	F	411	HIS	2.3
3	D	1292	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
5	F	410	TYR	2.2
5	F	322	GLY	2.2
2	C	158	TYR	2.2
2	C	196	LEU	2.2
5	F	362	SER	2.2
3	D	305	ALA	2.2
5	F	365	GLU	2.2
3	D	432	TYR	2.1
2	C	319	GLY	2.1
3	D	687	VAL	2.1
2	C	320	HIS	2.1
3	D	410	SER	2.1
5	F	388	ALA	2.1
3	D	220	ARG	2.1
5	F	380	GLU	2.0
5	F	371	LEU	2.0
5	F	387	GLY	2.0
2	C	529	VAL	2.0
2	C	409	ARG	2.0
5	F	382	THR	2.0
3	D	972	LEU	2.0
3	D	1294	VAL	2.0
5	F	398	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	MG	D	1601	1/1	0.74	0.28	71,71,71,71	0
10	POP	D	1602	9/9	0.77	0.08	69,80,94,96	0
9	MG	D	1603	1/1	0.98	0.09	50,50,50,50	0
11	ZN	D	1604	1/1	0.99	0.04	116,116,116,116	0
11	ZN	D	1605	1/1	0.99	0.10	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.