



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 01:31 am BST

PDB ID : 6OW3
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 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
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

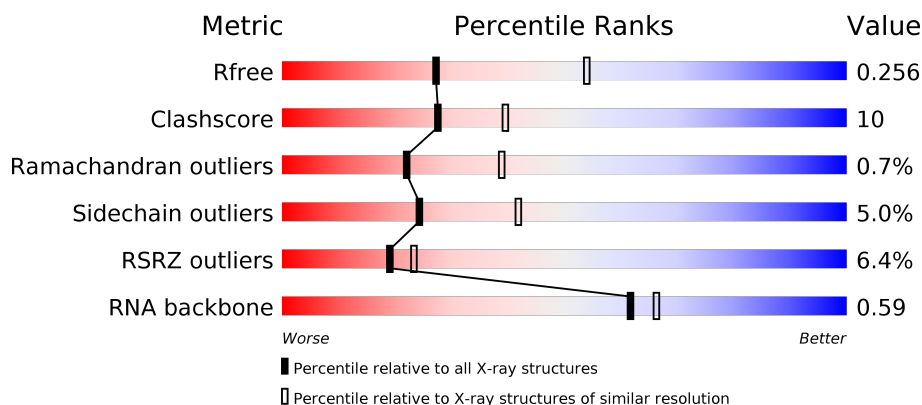
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	315	<div> <div>6%</div> <div>54%</div> <div>16%</div> <div>•</div> <div>28%</div> </div>
1	B	315	<div> <div>52%</div> <div>18%</div> <div>•</div> <div>29%</div> </div>
2	C	1119	<div> <div>6%</div> <div>72%</div> <div>25%</div> <div>••</div> </div>
3	D	1524	<div> <div>6%</div> <div>73%</div> <div>22%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div></div><div>3%</div><div>77%</div><div>18%</div><div>5%</div></div>
5	F	423	<div><div></div><div>13%</div><div>61%</div><div>19%</div><div>18%</div></div>
6	G	22	<div><div></div><div>23%</div><div>41%</div><div>9%</div><div>27%</div></div>
7	H	27	<div><div></div><div>7%</div><div>37%</div><div>33%</div><div>30%</div></div>
8	I	4	<div><div></div><div>25%</div><div>50%</div><div>25%</div></div>

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			

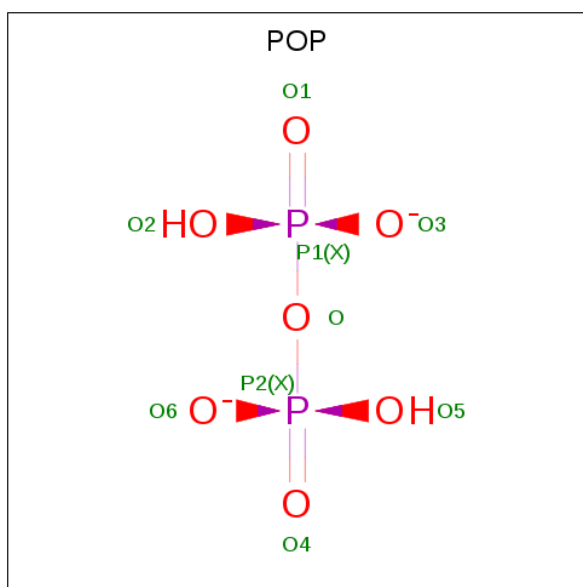
- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*G)-3').

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 (three-letter code: MG) (formula: Mg).

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

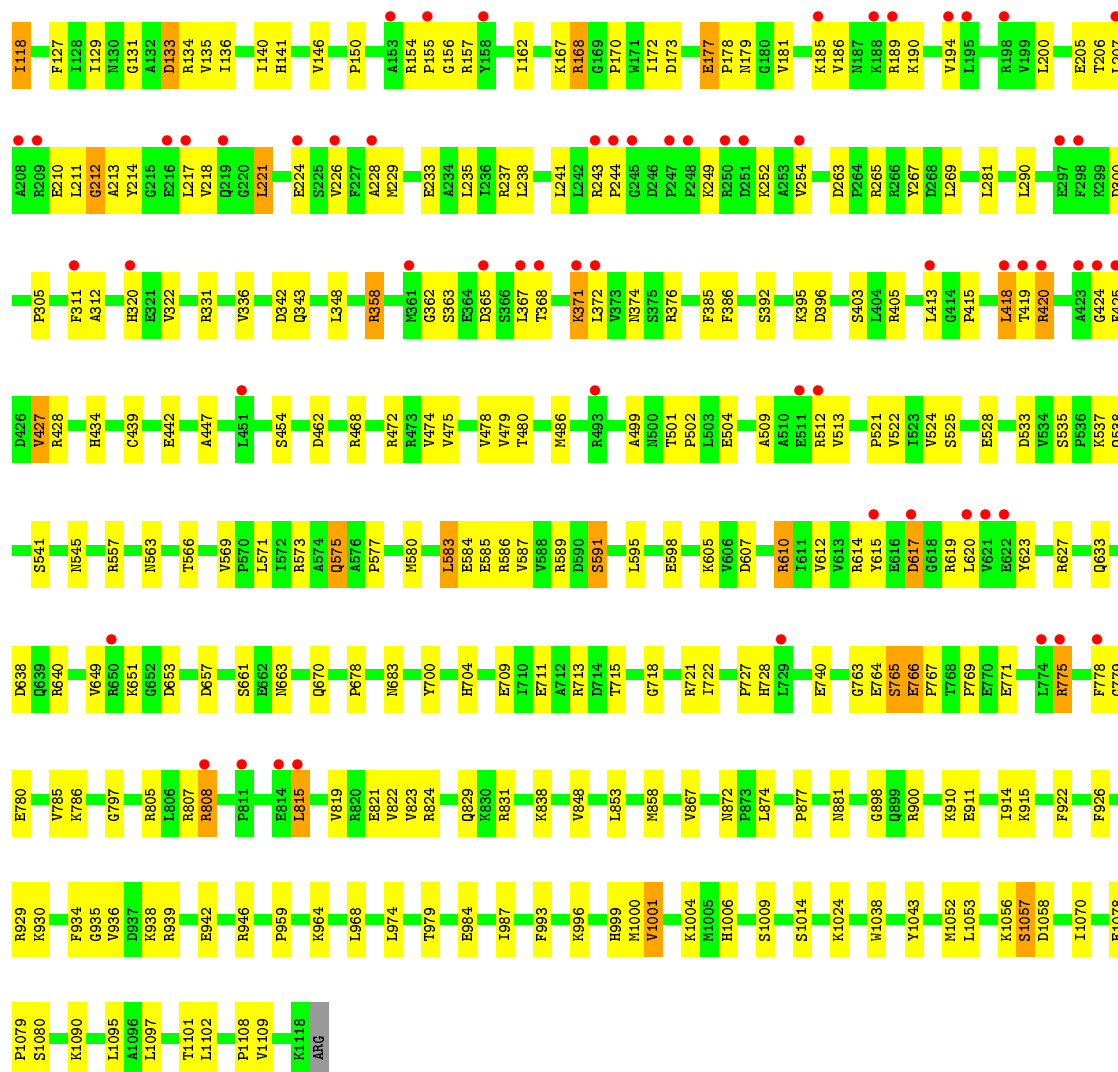
- Molecule 10 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



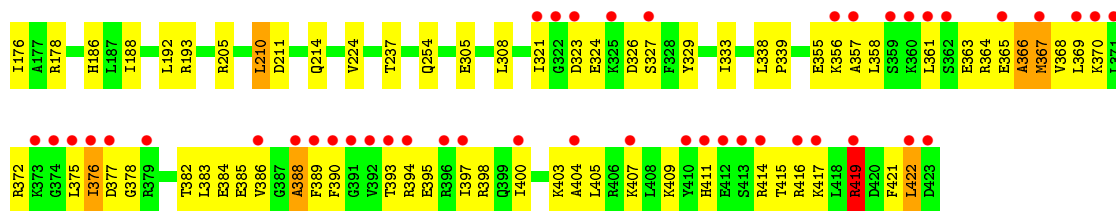
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

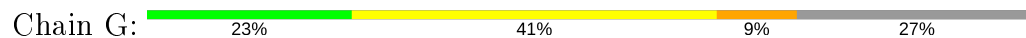
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		







- 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) 97.4 (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 , 0.256	Depositor DCC
R_{free} test set	2006 reflections (1.47%)	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 , 53.2	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

5.1 Standard geometry

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

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	0.55	0/1814	0.82	1/2466 (0.0%)
1	B	0.51	0/1799	0.78	0/2447
2	C	0.52	0/8925	0.80	3/12073 (0.0%)
3	D	0.57	1/11928 (0.0%)	0.83	7/16127 (0.0%)
4	E	0.48	0/775	0.76	0/1045
5	F	0.51	0/2852	0.89	5/3837 (0.1%)
6	G	1.41	4/367 (1.1%)	1.45	11/563 (2.0%)
7	H	1.01	0/439	1.10	1/675 (0.1%)
8	I	1.75	2/77 (2.6%)	1.40	0/119
All	All	0.57	7/28976 (0.0%)	0.84	28/39352 (0.1%)

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

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	3	G	O3'-P	-9.75	1.49	1.61
6	G	14	DG	N9-C4	-9.26	1.30	1.38
3	D	734	GLU	CG-CD	5.93	1.60	1.51
6	G	14	DG	N3-C4	-5.80	1.31	1.35
8	I	4	G	O3'-P	-5.49	1.54	1.61
6	G	14	DG	C1'-N9	-5.25	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	18	DT	N3-C4	5.02	1.42	1.38

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	13	DA	O5'-P-OP2	-10.32	96.42	105.70
6	G	16	DC	O5'-P-OP2	-9.40	97.24	105.70
5	F	422	LEU	CB-CG-CD2	8.66	125.73	111.00
6	G	13	DA	O5'-P-OP1	8.04	120.35	110.70
3	D	739	ASP	CB-CG-OD1	-7.68	111.39	118.30
3	D	1305	LEU	CA-CB-CG	7.28	132.04	115.30
6	G	16	DC	O4'-C4'-C3'	-7.18	101.63	104.50
3	D	583	ASP	CB-CG-OD2	-7.14	111.88	118.30
5	F	378	GLY	N-CA-C	-7.04	95.50	113.10
7	H	5	DA	O4'-C1'-N9	7.01	112.91	108.00
5	F	375	LEU	CA-CB-CG	6.75	130.81	115.30
2	C	107	LEU	CA-CB-CG	6.66	130.62	115.30
6	G	15	DC	O5'-P-OP2	-6.51	99.84	105.70
3	D	46	ASP	CB-CG-OD1	5.97	123.67	118.30
3	D	739	ASP	N-CA-CB	5.96	121.33	110.60
6	G	14	DG	N3-C4-N9	-5.94	122.44	126.00
5	F	419	ARG	CA-CB-CG	5.80	126.16	113.40
3	D	783	ARG	NE-CZ-NH2	-5.73	117.44	120.30
6	G	17	DC	O4'-C4'-C3'	-5.56	102.28	104.50
3	D	1363	LEU	CA-CB-CG	5.52	127.99	115.30
6	G	18	DT	N3-C4-O4	5.51	123.20	119.90
6	G	11	DA	O4'-C1'-N9	5.25	111.68	108.00
2	C	371	LYS	CA-CB-CG	5.16	124.75	113.40
1	A	219	ARG	NE-CZ-NH2	-5.15	117.72	120.30
6	G	17	DC	O5'-P-OP2	-5.13	101.08	105.70
2	C	765	SER	CA-C-N	-5.12	105.93	117.20
6	G	15	DC	OP1-P-OP2	5.11	127.27	119.60
5	F	388	ALA	N-CA-C	5.05	124.64	111.00

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

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Mol	Chain	Res	Type	Group
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	1833	40	0
1	B	1767	0	1816	38	0
2	C	8758	0	8852	219	0
3	D	11722	0	11950	234	1
4	E	761	0	778	15	0
5	F	2807	0	2882	71	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	28552	567	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 (567) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:658:LEU:HD23	3:D:661:MET:HE3	1.72	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
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.76	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
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD2	3:D:1314:LYS:H	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
2:C:853:LEU:HB2	2:C:858:MET:CE	2.27	0.64
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
5:F:383:LEU:HD22	5:F:394:ARG:HH22	1.62	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
6:G:19:DA:H2'	6:G:20:DA:C8	2.34	0.62
2:C:1078:GLU:HG2	2:C:1079:PRO:HD2	1.81	0.62
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.81	0.62
2:C:425:PHE:CD1	3:D:1079:LYS:HE3	2.35	0.62
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.82	0.61
1:B:65:PHE:CD2	3:D:809:PRO:HB2	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	5:F:414:ARG:HB3	1.66	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
2:C:764:GLU:C	2:C:766:GLU:H	2.03	0.60
3:D:1277:ILE:HG13	3:D:1278:ASP:H	1.66	0.60
3:D:1100:ASP:OD1	3:D:1463:LYS:NZ	2.27	0.59
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: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
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
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: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
2:C:167:LYS:NZ	7:H:11:DG:H5"	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH2	2:C:420:ARG:HB2	2.20	0.56
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
6:G:18:DT:H2'	6:G:19:DA:C8	2.41	0.55
6:G:20:DA:H5"	6:G:20:DA:H8	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
2:C:129:ILE:HG12	2:C:386:PHE:HB3	1.88	0.55
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.40	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:702:LEU:HB3	3:D:745:MET:HE2	1.88	0.54
3:D:1444:THR:O	3:D:1448:THR:HG23	2.07	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
2:C:74:GLY:HA3	2:C:93:PRO:HG2	1.87	0.54
3:D:1152:GLU:OE1	3:D:1161:GLU:HA	2.08	0.54
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.90	0.54
3:D:860:LEU:O	3:D:876:SER:HB2	2.07	0.54
3:D:693:GLU:HA	4:E:48:MET:HE3	1.89	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:1126:ASP:O	3:D:1130:ARG:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:763:GLY:C	2:C:765:SER:H	2.11	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
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.43	0.53
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.09	0.53
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.44	0.53
3:D:750:PRO:O	3:D:756:GLN:NE2	2.42	0.53
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.44	0.53
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.41	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1043:TYR:CD2	3:D:763:MET:HG2	2.46	0.50
2:C:229:MET:HB2	2:C:233:GLU:CB	2.39	0.50
3:D:949:ILE:HD11	3:D:1023:MET:HE1	1.94	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:1102:LEU:HD23	2:C:1108:PRO:HA	1.94	0.50
2:C:168:ARG:NH2	2:C:265:ARG:O	2.45	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
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:396:ASP:HA	2:C:633:GLN:NE2	2.27	0.49
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.95	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:1480:PHE:O	4:E:18:ARG:NH2	2.46	0.49
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:1291:SER:OG	3:D:1304:LYS:HG2	2.13	0.48
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.94	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
3:D:1108:ARG:HD2	3:D:1198:TYR:O	2.14	0.48
5:F:394:ARG:HG3	5:F:395:GLU:N	2.29	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:1093:TYR:OH	3:D:1441:GLN:OE1	2.28	0.48
3:D:922:LEU:HB3	3:D:926:LYS:HD2	1.96	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
1:B:70:GLY:O	1:B:133:GLU:HG3	2.14	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:1263:PHE:HD2	3:D:1375:MET:CE	2.27	0.47
3:D:1198:TYR:CZ	3:D:1460:ILE:HD13	2.49	0.47
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.96	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
5:F:366:ALA:O	5:F:370:LYS:HB2	2.14	0.47
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.49	0.47
2:C:374:ASN:OD1	2:C:376:ARG:HG2	2.14	0.47
5:F:127:ILE:O	5:F:131:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASP:OD1	2:C:938:LYS:NZ	2.46	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
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.97	0.47
2:C:1095:LEU:HD23	3:D:582:LEU:HD22	1.96	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: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
3:D:258:VAL:HG12	3:D:273:ARG:O	2.15	0.47
5:F:414:ARG:HB3	5:F:414:ARG:NH1	2.29	0.47
3:D:573:MET:HE1	5:F:214:GLN:HG3	1.96	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:243:ARG:NH1	7:H:10:DA:N1	2.62	0.47
2:C:263:ASP:C	2:C:265:ARG:H	2.18	0.47
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.97	0.47
2:C:420:ARG:NE	8:I:2:GTP:O1B	2.48	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:1087:ARG:HG3	3:D:1256:LEU:HD23	1.98	0.46
3:D:134:VAL:HG23	3:D:149:LYS:HA	1.97	0.46
3:D:1236:LEU:HG	3:D:1359:GLN:HG3	1.98	0.46
3:D:134:VAL:CG2	3:D:151:GLN:H	2.28	0.46
3:D:638:LYS:HD3	3:D:638:LYS:HA	1.74	0.46
3:D:671:LYS:HE3	5:F:421:PHE:HA	1.97	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:77:PRO:HB2	2:C:78:PHE:CD1	2.51	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:329:TYR:CE2	5:F:333:ILE:HD11	2.51	0.45
5:F:393:THR:HG22	5:F:394:ARG:N	2.31	0.45
5:F:82:ARG:HB2	7:H:8:DG:O6	2.16	0.45
2:C:185:LYS:HE2	2:C:190:LYS:HE3	1.97	0.45
2:C:229:MET:HE3	2:C:237:ARG:NH2	2.31	0.45
2:C:974:LEU:HA	2:C:974:LEU:HD12	1.64	0.45
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.55	0.45
2:C:617:ASP:HB2	2:C:619:ARG:HG2	1.97	0.45
3:D:1217:ILE:HD12	3:D:1480:PHE:CZ	2.51	0.45
3:D:632:VAL:O	3:D:727:GLN:HA	2.16	0.45
3:D:1154:GLU:OE2	3:D:1159:ARG:HB2	2.16	0.45
3:D:741:ASP:OD1	3:D:743:ASP:OD1	2.35	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:C8	8:I:2:GTP:O1A	2.70	0.45
3:D:1092:GLY:HA3	6:G:14:DG:O4'	2.17	0.45
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.99	0.45
3:D:1290:LEU:HB3	3:D:1305:LEU:HD23	1.99	0.45
2:C:177:GLU:HG3	2:C:178:PRO:HD2	2.00	0.44
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.98	0.44
3:D:1277:ILE:HG13	3:D:1278:ASP:N	2.31	0.44
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.98	0.44
1:B:185:ARG:NH1	1:B:187:GLY:O	2.50	0.44
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:815:LEU:HD23	2:C:819:VAL:CG1	2.41	0.44
3:D:1263:PHE:O	3:D:1375:MET:HE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:74:GLU:H	3:D:74:GLU:CD	2.21	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: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
3:D:1283:ILE:HG12	3:D:1315:ASP:CG	2.38	0.44
4:E:36:LYS:CG	4:E:93:TYR:HB3	2.47	0.44
2:C:135:VAL:HG23	2:C:395:LYS:HG3	2.00	0.44
2:C:224:GLU:CD	2:C:224:GLU:H	2.22	0.44
2:C:418:LEU:HD12	2:C:418:LEU:H	1.82	0.44
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.53	0.44
8:I:2:GTP:H8	8:I:2:GTP:O5'	2.01	0.44
1:B:153:ALA:C	1:B:155:LYS:H	2.21	0.43
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
2:C:580:MET:HB3	2:C:584:GLU:CD	2.38	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:405:ARG:HG2	2:C:405:ARG:O	2.17	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
2:C:911:GLU:CD	3:D:1062:ARG:HH11	2.22	0.43
3:D:351:MET:HG2	3:D:370:ALA:HB2	2.00	0.43
1:A:216:GLU:CD	1:A:219:ARG:HH22	2.22	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
3:D:1089:ALA:HA	6:G:14:DG:C8	2.54	0.43
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.83	0.43
3:D:1402:ALA:O	3:D:1406:ARG:HG3	2.18	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:HA	3:D:972:LEU:HD13	1.61	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
5:F:415:THR:C	5:F:417:LYS:H	2.21	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:11:PHE:O	1:B:228:PRO:HA	2.18	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
5:F:148:LYS:HB2	5:F:148:LYS:HE3	1.74	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
2:C:763:GLY:C	2:C:765:SER:N	2.72	0.43
2:C:3:ILE:HD13	2:C:900:ARG:HB2	2.01	0.43
3:D:405:ASP:CG	3:D:406:ASP:H	2.23	0.43
1:B:38:ASN:OD1	2:C:979:THR:HG22	2.19	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
2:C:569:VAL:HG21	2:C:1000:MET:HE3	2.01	0.42
1:A:180:GLN:NE2	2:C:935:GLY:O	2.51	0.42
3:D:17:LYS:HB2	3:D:17:LYS:HE2	1.68	0.42
3:D:526:PRO:HB2	3:D:528:VAL:HG13	2.00	0.42
3:D:65:ARG:HB2	5:F:377:ASP:O	2.19	0.42
3:D:949:ILE:HD11	3:D:1023:MET:CE	2.49	0.42
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.00	0.42
2:C:167:LYS:HZ1	7:H:11:DG:H5"	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.38	0.42
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.55	0.42
3:D:658:LEU:HA	3:D:661:MET:HE2	2.01	0.42
3:D:882:PHE:HE1	3:D:900:ILE:HG23	1.84	0.42
5:F:358:LEU:O	5:F:366:ALA:HB2	2.20	0.42
5:F:81:VAL:HG22	5:F:210:LEU:CD1	2.49	0.42
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	2.01	0.42
2:C:269:LEU:HA	2:C:269:LEU:HD12	1.79	0.42
2:C:69:LEU:HB2	2:C:97:ARG:O	2.19	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:185:LYS:HB2	2:C:185:LYS:HE2	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:167:LYS:HZ3	7:H:11:DG:H5"	1.85	0.42
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.34	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
3:D:131:LYS:N	3:D:456:MET:HE2	2.35	0.42
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.19	0.42
1:A:61:VAL:HG21	1:A:68:ILE:HD11	2.02	0.42
2:C:1009:SER:HB3	3:D:651:GLU:O	2.19	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:877:PRO:HG3	3:D:1023:MET:HE1	2.01	0.42
3:D:1420:LEU:HA	3:D:1420:LEU:HD12	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:HA	3:D:618:LEU:HD13	1.89	0.42
4:E:48:MET:HE2	4:E:50:THR:HG22	2.01	0.42
1:A:25:LEU:HA	1:A:25:LEU:HD12	1.86	0.41
2:C:200:LEU:HD13	2:C:300:ASP:HB2	2.00	0.41
2:C:56:GLU:HG2	2:C:64:LEU:HB2	2.02	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:HA	5:F:166:LEU:HD23	1.88	0.41
1:A:101:LEU:HD21	1:A:109:VAL:HG11	2.02	0.41
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:LEU:HA	3:D:12:LEU:HD23	1.85	0.41
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.55	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
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
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:996:LYS:HE2	2:C:1000:MET:CE	2.50	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
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.20	0.41
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	2.02	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
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
3:D:288:MET:HA	3:D:306:GLU:O	2.20	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
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
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
2:C:211:LEU:HD23	2:C:311:PHE:CD2	2.53	0.41
2:C:133:ASP:HB3	2:C:395:LYS:HD2	2.02	0.41
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.23	0.41
5:F:355:GLU:C	5:F:357:ALA:H	2.23	0.41
1:A:20:TYR:C	1:A:207:PRO:HG2	2.41	0.41
1:B:162:ILE:O	1:B:163:ASN:HB2	2.21	0.41
3:D:34:TYR:CZ	3:D:35:ARG:HG3	2.56	0.41
3:D:65:ARG:NH1	5:F:376:ILE:HA	2.36	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1053:LEU:HA	3:D:621:LYS:HD2	2.03	0.40
2:C:238:LEU:O	2:C:241:LEU:HB2	2.22	0.40
2:C:32:ALA:HB2	2:C:73:LEU:HD12	2.04	0.40
5:F:321:ILE:HG23	5:F:321:ILE:HD12	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:778:PHE:C	2:C:780:GLU:H	2.24	0.40
3:D:387:LEU:HA	3:D:387:LEU:HD23	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:HD12	2:C:348:LEU:HA	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%)	29	47
2	C	1107/1119 (99%)	1062 (96%)	36 (3%)	9 (1%)	19	34
3	D	1480/1524 (97%)	1434 (97%)	39 (3%)	7 (0%)	29	47
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	14	25
5	F	344/423 (81%)	319 (93%)	18 (5%)	7 (2%)	7	13
All	All	3469/3795 (91%)	3334 (96%)	110 (3%)	25 (1%)	22	39

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
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 ⓘ

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%)	189 (95%)	10 (5%)	24	42
1	B	197/273 (72%)	187 (95%)	10 (5%)	24	41
2	C	934/941 (99%)	889 (95%)	45 (5%)	25	44
3	D	1250/1279 (98%)	1183 (95%)	67 (5%)	22	38
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	55
5	F	301/371 (81%)	288 (96%)	13 (4%)	29	48
All	All	2964/3225 (92%)	2816 (95%)	148 (5%)	24	42

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	VAL
1	A	104	GLU
1	A	133	GLU
1	A	134	GLU
1	A	184	THR
1	A	186	LEU
1	A	189	ARG
1	A	205	VAL
1	A	206	THR
1	A	229	GLN
1	B	14	ARG
1	B	34	VAL
1	B	38	ASN
1	B	112	ARG
1	B	126	ASP
1	B	134	GLU
1	B	183	ASP
1	B	186	LEU
1	B	190	THR
1	B	206	THR
2	C	8	ARG
2	C	15	LEU

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Mol	Chain	Res	Type
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	141	HIS
2	C	168	ARG
2	C	177	GLU
2	C	194	VAL
2	C	205	GLU
2	C	221	LEU
2	C	342	ASP
2	C	358	ARG
2	C	413	LEU
2	C	420	ARG
2	C	427	VAL
2	C	434	HIS
2	C	454	SER
2	C	522	VAL
2	C	525	SER
2	C	557	ARG
2	C	575	GLN
2	C	583	LEU
2	C	585	GLU
2	C	586	ARG
2	C	591	SER
2	C	610	ARG
2	C	617	ASP
2	C	640	ARG
2	C	661	SER
2	C	775	ARG
2	C	786	LYS
2	C	808	ARG
2	C	815	LEU
2	C	848	VAL
2	C	939	ARG
2	C	942	GLU
2	C	968	LEU
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER

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Mol	Chain	Res	Type
2	C	1080	SER
3	D	30	GLU
3	D	67	ARG
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	190	GLU
3	D	191	LEU
3	D	198	ARG
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	273	ARG
3	D	276	ASP
3	D	312	ARG
3	D	362	GLU
3	D	372	ASP
3	D	411	THR
3	D	421	LEU
3	D	423	ASP
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	650	LEU
3	D	709	HIS
3	D	739	ASP
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	813	LEU
3	D	817	GLU
3	D	864	VAL
3	D	875	THR
3	D	904	VAL

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Mol	Chain	Res	Type
3	D	907	GLU
3	D	970	LYS
3	D	972	LEU
3	D	997	THR
3	D	1041	LEU
3	D	1062	ARG
3	D	1130	ARG
3	D	1155	VAL
3	D	1188	VAL
3	D	1195	GLN
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
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	1493	LYS
4	E	8	LYS
4	E	66	LYS
4	E	75	PHE
5	F	98	GLU
5	F	125	ASP
5	F	159	ILE
5	F	186	HIS
5	F	205	ARG
5	F	210	LEU
5	F	211	ASP
5	F	254	GLN
5	F	326	ASP
5	F	367	MET
5	F	372	ARG
5	F	376	ILE
5	F	419	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	B	63	HIS
2	C	683	ASN
2	C	728	HIS
3	D	388	HIS
3	D	714	GLN
3	D	724	GLN
3	D	737	ASN
3	D	744	GLN
5	F	83	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 carbohydrates 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	0.86	0	13,13,13	0.94	1 (7%)

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.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
10	D	1602	POP	P2-O-P1	-2.32	124.86	132.83

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%)	0.03	2 (0%) 84 89	65, 88, 111, 123	0
1	B	224/315 (71%)	0.11	1 (0%) 92 95	63, 90, 120, 134	0
2	C	1111/1119 (99%)	0.38	69 (6%) 20 25	50, 87, 154, 180	0
3	D	1484/1524 (97%)	0.35	93 (6%) 20 24	45, 81, 145, 175	0
4	E	94/99 (94%)	0.42	3 (3%) 47 56	60, 98, 137, 147	0
5	F	346/423 (81%)	0.90	55 (15%) 1 2	56, 97, 180, 196	0
6	G	16/22 (72%)	-0.04	0 100 100	56, 92, 179, 180	0
7	H	19/27 (70%)	-0.00	2 (10%) 6 7	82, 125, 162, 166	0
8	I	3/4 (75%)	-1.02	0 100 100	58, 58, 64, 73	0
All	All	3523/3848 (91%)	0.38	225 (6%) 19 23	45, 87, 154, 196	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	375	LEU	11.9
5	F	392	VAL	11.7
5	F	376	ILE	11.6
5	F	390	PHE	10.0
5	F	393	THR	10.0
5	F	410	TYR	8.8
5	F	397	ILE	8.0
5	F	325	LYS	6.6
5	F	360	LYS	6.5
5	F	389	PHE	6.1
3	D	409	VAL	6.0
5	F	361	LEU	5.9
5	F	356	LYS	5.9
5	F	370	LYS	5.5
5	F	414	ARG	5.4

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Mol	Chain	Res	Type	RSRZ
2	C	207	LEU	5.4
5	F	371	LEU	5.2
5	F	367	MET	5.2
3	D	68	PHE	5.1
3	D	1497	GLU	5.0
2	C	245	GLY	5.0
2	C	107	LEU	5.0
5	F	396	ARG	5.0
2	C	188	LYS	4.9
4	E	85	LEU	4.9
5	F	357	ALA	4.9
5	F	386	VAL	4.8
5	F	391	GLY	4.8
5	F	374	GLY	4.8
2	C	423	ALA	4.7
5	F	149	GLU	4.6
4	E	32	ARG	4.6
3	D	310	LEU	4.4
3	D	371	ILE	4.3
3	D	980	MET	4.3
5	F	400	ILE	4.3
5	F	359	SER	4.3
5	F	394	ARG	4.2
2	C	814	GLU	4.2
2	C	297	GLU	4.2
5	F	404	ALA	4.1
5	F	417	LYS	4.1
5	F	362	SER	4.1
5	F	323	ASP	4.1
2	C	367	LEU	4.0
5	F	422	LEU	3.9
3	D	486	ARG	3.9
5	F	412	GLU	3.9
3	D	1128	VAL	3.8
2	C	217	LEU	3.8
3	D	211	VAL	3.8
3	D	983	LEU	3.7
5	F	369	LEU	3.7
3	D	173	PRO	3.7
2	C	208	ALA	3.7
3	D	1129	THR	3.7
3	D	198	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	99	LEU	3.7
2	C	64	LEU	3.6
5	F	379	ARG	3.6
5	F	141	VAL	3.6
3	D	1318	TYR	3.6
5	F	377	ASP	3.6
3	D	1493	LYS	3.6
2	C	815	LEU	3.5
5	F	416	ARG	3.5
3	D	216	VAL	3.5
2	C	650	ARG	3.5
3	D	974	ILE	3.4
3	D	1499	ARG	3.4
5	F	388	ALA	3.4
3	D	1294	VAL	3.4
2	C	298	PHE	3.4
3	D	1502	ALA	3.3
3	D	1312	LEU	3.3
2	C	424	GLY	3.3
5	F	407	LYS	3.3
5	F	159	ILE	3.3
3	D	488	ARG	3.3
3	D	1327	ARG	3.3
5	F	147	LEU	3.3
2	C	155	PRO	3.3
1	B	16	GLN	3.3
3	D	1490	LYS	3.3
2	C	194	VAL	3.3
2	C	189	ARG	3.3
2	C	811	PRO	3.2
3	D	220	ARG	3.2
3	D	188	GLY	3.2
3	D	1305	LEU	3.2
2	C	365	ASP	3.2
2	C	195	LEU	3.2
5	F	148	LYS	3.2
2	C	228	ALA	3.2
2	C	620	LEU	3.2
3	D	1299	PHE	3.1
3	D	379	ALA	3.1
7	H	11	DG	3.1
2	C	413	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	66	LEU	3.1
5	F	151	LEU	3.1
3	D	152	LEU	3.1
2	C	251	ASP	3.0
5	F	365	GLU	3.0
2	C	209	ARG	3.0
3	D	971	LEU	2.9
5	F	413	SER	2.9
2	C	368	THR	2.9
2	C	153	ALA	2.9
2	C	102	HIS	2.9
2	C	216	GLU	2.9
2	C	617	ASP	2.9
2	C	808	ARG	2.9
2	C	729	LEU	2.8
2	C	511	GLU	2.8
3	D	178	LEU	2.8
3	D	485	SER	2.8
2	C	250	ARG	2.8
3	D	63	TYR	2.8
5	F	173	TYR	2.8
5	F	411	HIS	2.8
3	D	832	ARG	2.8
3	D	1313	VAL	2.7
3	D	343	LYS	2.7
3	D	487	ALA	2.7
4	E	89	MET	2.7
2	C	104	ASP	2.7
5	F	143	HIS	2.7
3	D	268	ALA	2.7
3	D	241	ILE	2.7
2	C	320	HIS	2.7
3	D	142	LEU	2.7
2	C	615	TYR	2.6
3	D	1298	GLY	2.6
2	C	109	LYS	2.6
3	D	316	GLN	2.6
3	D	377	VAL	2.6
2	C	224	GLU	2.6
3	D	236	TYR	2.6
2	C	778	PHE	2.6
2	C	10	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
5	F	419	ARG	2.6
3	D	345	TYR	2.5
2	C	425	PHE	2.5
3	D	336	PHE	2.5
3	D	1310	ARG	2.5
3	D	1488	ASP	2.5
2	C	372	LEU	2.5
3	D	427	VAL	2.5
2	C	158	TYR	2.5
2	C	254	VAL	2.5
3	D	368	VAL	2.5
5	F	423	ASP	2.5
3	D	360	ARG	2.4
2	C	419	THR	2.4
5	F	150	THR	2.4
2	C	418	LEU	2.4
3	D	1290	LEU	2.4
5	F	142	ARG	2.4
2	C	100	LEU	2.4
3	D	1311	LEU	2.4
3	D	147	VAL	2.4
3	D	428	LYS	2.4
3	D	1086	LEU	2.4
2	C	621	VAL	2.4
3	D	196	VAL	2.4
3	D	287	GLY	2.4
3	D	1307	LYS	2.4
3	D	1319	VAL	2.4
2	C	219	GLN	2.3
3	D	432	TYR	2.3
3	D	1292	VAL	2.3
2	C	451	LEU	2.3
3	D	1308	GLU	2.3
3	D	213	VAL	2.3
3	D	1130	ARG	2.3
2	C	248	PRO	2.3
3	D	1414	PRO	2.3
3	D	170	PRO	2.3
3	D	1300	SER	2.3
3	D	1500	LYS	2.3
3	D	1287	GLU	2.3
2	C	420	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	774	LEU	2.2
3	D	193	PRO	2.2
3	D	165	LYS	2.2
3	D	490	ALA	2.2
2	C	185	LYS	2.2
7	H	15	DT	2.2
2	C	493	ARG	2.2
2	C	243	ARG	2.2
2	C	247	PRO	2.2
3	D	320	ALA	2.2
2	C	198	ARG	2.2
2	C	311	PHE	2.2
2	C	371	LYS	2.2
3	D	194	GLY	2.2
3	D	237	LYS	2.1
3	D	978	TYR	2.1
3	D	317	VAL	2.1
3	D	1278	ASP	2.1
2	C	775	ARG	2.1
3	D	1281	VAL	2.1
3	D	393	ILE	2.1
3	D	190	GLU	2.1
3	D	1436	SER	2.1
3	D	67	ARG	2.1
5	F	373	LYS	2.1
2	C	226	VAL	2.1
5	F	321	ILE	2.1
2	C	512	ARG	2.1
3	D	41	ARG	2.1
1	A	94	LEU	2.1
2	C	361	MET	2.1
2	C	622	GLU	2.1
5	F	327	SER	2.1
5	F	322	GLY	2.1
3	D	144	GLY	2.0
3	D	1405	GLU	2.0
3	D	1495	ILE	2.0
3	D	62	LYS	2.0
3	D	189	GLN	2.0
3	D	808	THR	2.0
3	D	375	GLU	2.0
2	C	244	PRO	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 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
9	MG	D	1601	1/1	0.89	0.51	71,71,71,71	0
10	POP	D	1602	9/9	0.94	0.25	69,80,94,96	0
9	MG	D	1603	1/1	0.96	0.21	50,50,50,50	0
11	ZN	D	1604	1/1	0.96	0.11	116,116,116,116	0
11	ZN	D	1605	1/1	0.99	0.24	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.