



Full wwPDB X-ray Structure Validation Report ⓘ

May 30, 2020 – 04:49 am BST

PDB ID : 6P70
Title : X-ray crystal structure of bacterial RNA polymerase and pyrBI promoter complex
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2019-06-04
Resolution : 3.05 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
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

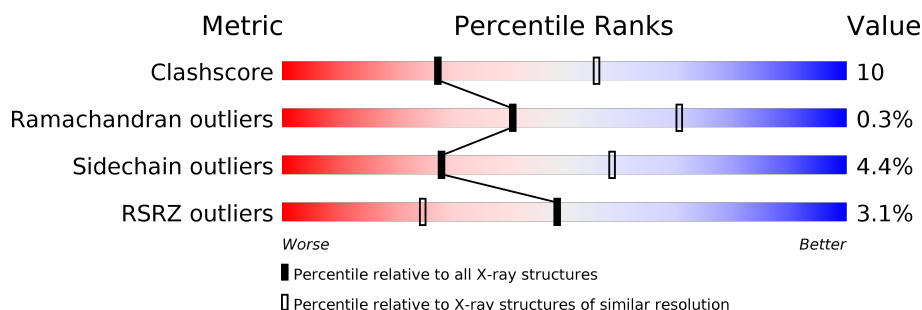
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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))
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	
5	F	423	
6	G	21	

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Mol	Chain	Length	Quality of chain
7	H	27	 <p>A horizontal bar chart showing the quality of chain H. The bar is divided into four segments: a small red segment at the beginning labeled '7%', followed by a green segment labeled '52%', a yellow segment labeled '30%', and a grey segment at the end labeled '19%'.</p>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28421 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	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	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
			8764	5545	1561	1634	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1486	Total	C	N	O	S	0	0	0
			11738	7440	2067	2195	36			

- 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*TP*CP*CP*CP*GP*GP*CP*AP*AP*AP*TP*TP*GP*TP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	18	Total	C	N	O	P	0	0	0
			364	173	64	109	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	22	Total	C	N	O	P	0	0	0
			450	216	81	132	21			

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	1	Total	Mg	0	0
			1	1		
8	B	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		

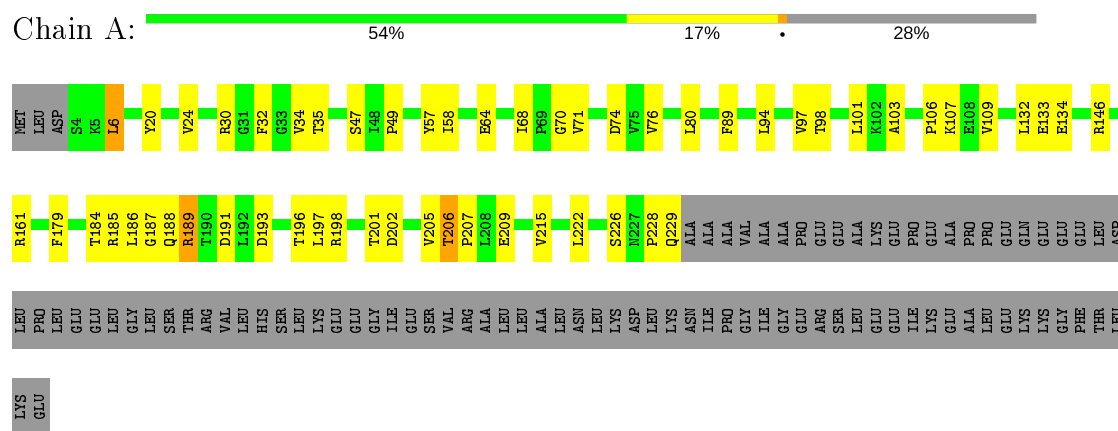
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

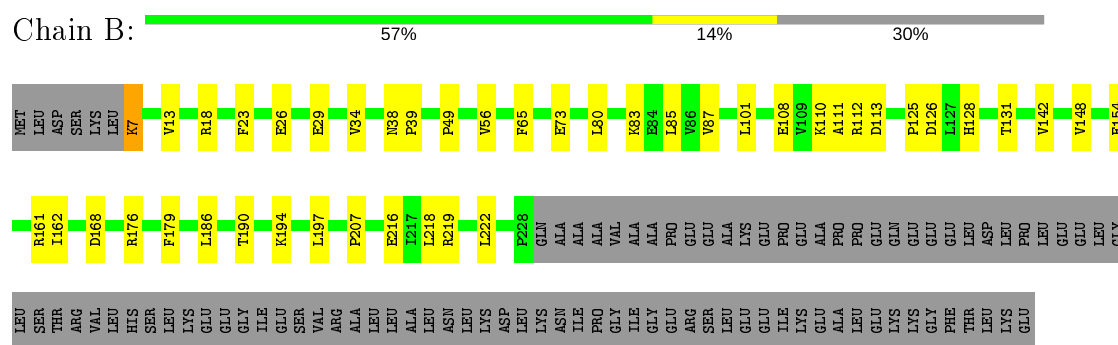
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

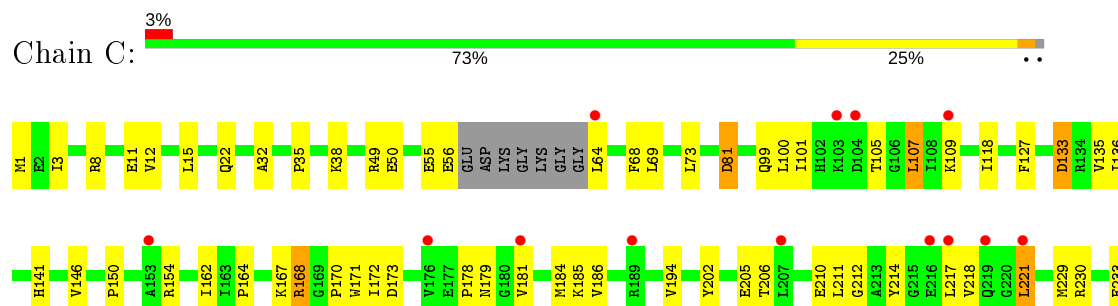
- Molecule 1: DNA-directed RNA polymerase subunit alpha

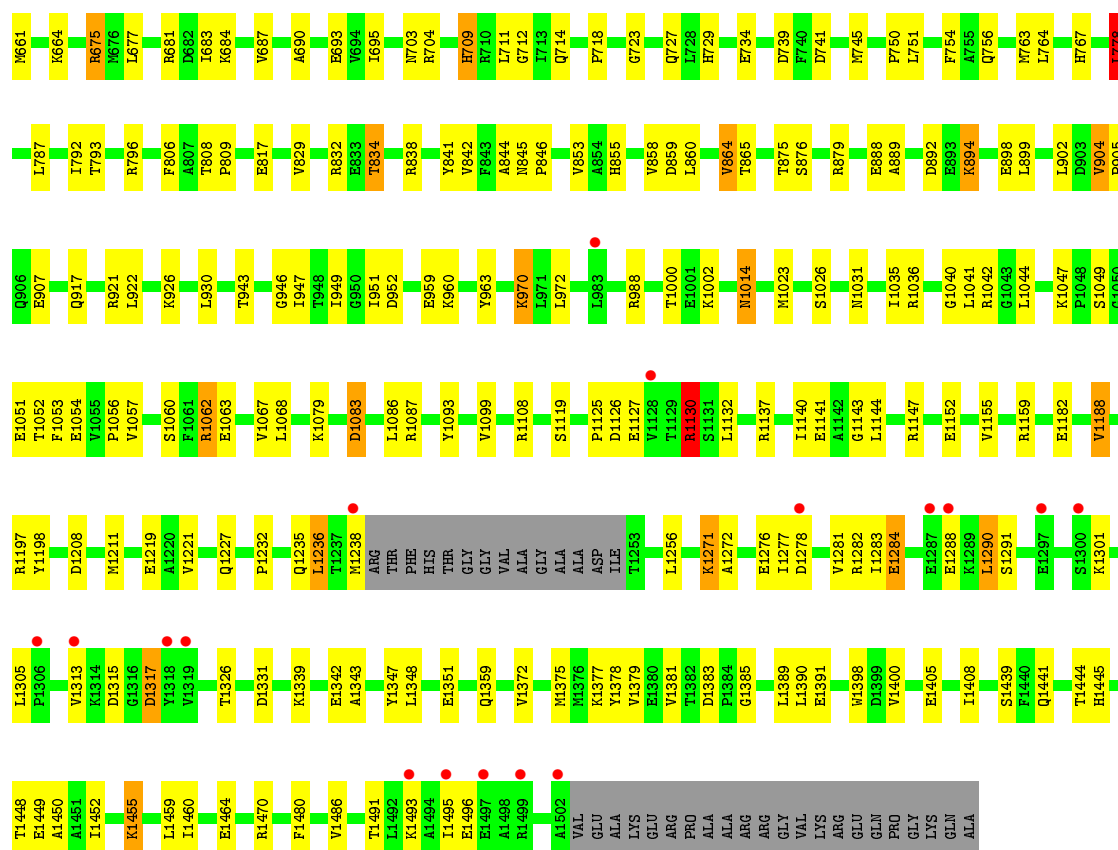


- Molecule 1: DNA-directed RNA polymerase subunit alpha



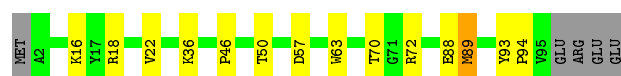
- Molecule 2: DNA-directed RNA polymerase subunit beta





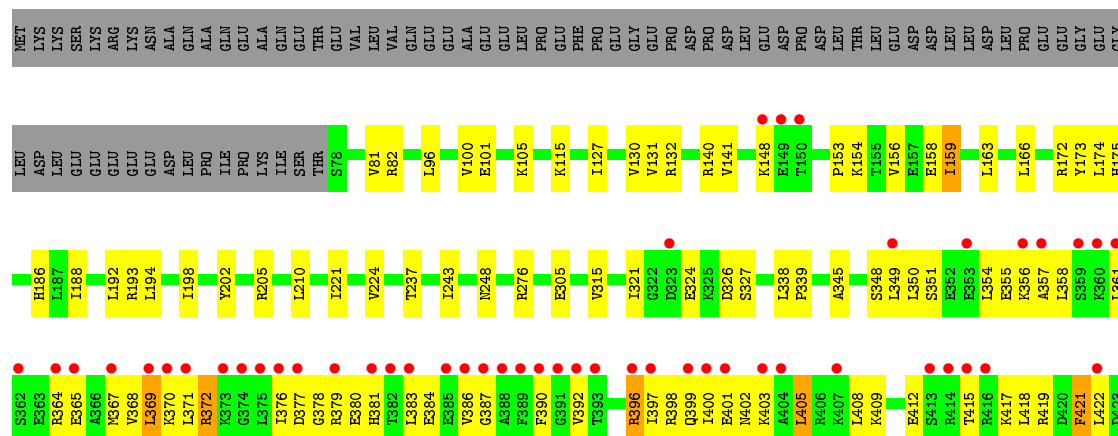
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 81% 13% • 5%

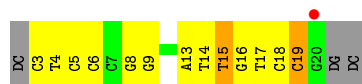


- Molecule 5: RNA polymerase sigma factor SigA

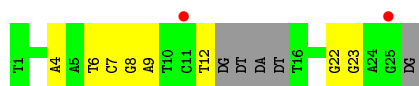
Chain F: 12% 59% 22% • 18%



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



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*CP*GP*AP*TP*CP*TP*TP*TP*GP*CP*CP*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	185.18Å 100.84Å 294.87Å 90.00° 98.81° 90.00°	Depositor
Resolution (Å)	46.06 – 3.05 46.06 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.06-3.05) 99.1 (46.06-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.06Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.207 , 0.252 (Not available) , (Not available)	Depositor DCC
R_{free} test set	2000 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28421	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.53	0/1814	0.75	0/2466
1	B	0.54	0/1782	0.75	0/2424
2	C	0.53	0/8931	0.78	4/12080 (0.0%)
3	D	0.57	2/11944 (0.0%)	0.82	6/16148 (0.0%)
4	E	0.49	0/775	0.76	0/1045
5	F	0.55	0/2852	0.83	5/3837 (0.1%)
6	G	1.22	1/406 (0.2%)	1.03	2/623 (0.3%)
7	H	1.42	1/503 (0.2%)	1.13	1/773 (0.1%)
All	All	0.59	4/29007 (0.0%)	0.81	18/39396 (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
3	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	23	DG	O3'-P	-17.21	1.40	1.61
6	G	19	DC	C1'-N1	7.03	1.58	1.49
3	D	156	GLU	CG-CD	6.07	1.61	1.51
3	D	734	GLU	CG-CD	5.23	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	23	DG	P-O3'-C3'	8.35	129.72	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	944	LEU	CB-CG-CD2	-7.53	98.20	111.00
6	G	15	DT	O4'-C4'-C3'	-7.04	101.68	104.50
2	C	775	ARG	CB-CG-CD	-6.94	93.55	111.60
5	F	405	LEU	CA-CB-CG	6.88	131.12	115.30
3	D	739	ASP	CB-CG-OD2	-6.01	112.89	118.30
5	F	369	LEU	CA-CB-CG	5.91	128.90	115.30
3	D	1086	LEU	CA-CB-CG	5.83	128.72	115.30
2	C	107	LEU	CA-CB-CG	5.78	128.60	115.30
5	F	396	ARG	NE-CZ-NH2	-5.72	117.44	120.30
3	D	583	ASP	CB-CG-OD1	5.71	123.44	118.30
5	F	396	ARG	CG-CD-NE	-5.63	99.98	111.80
3	D	778	LEU	CA-CB-CG	-5.32	103.07	115.30
3	D	1083	ASP	CB-CG-OD1	-5.30	113.53	118.30
2	C	460	ARG	CB-CA-C	5.27	120.94	110.40
3	D	739	ASP	CB-CG-OD1	5.20	122.98	118.30
5	F	387	GLY	C-N-CA	5.13	134.52	121.70
6	G	14	DT	O4'-C4'-C3'	-5.06	102.47	104.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	620	GLY	Mainchain

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	37	0
1	B	1750	0	1797	30	0
2	C	8764	0	8863	211	1
3	D	11738	0	11969	249	0
4	E	761	0	778	9	0
5	F	2807	0	2882	81	1
6	G	364	0	203	12	0
7	H	450	0	252	13	0
8	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	1	0	0	0	0
8	G	1	0	0	0	0
9	D	2	0	0	0	0
All	All	28421	0	28578	571	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 (571) 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)
2:C:775:ARG:HE	2:C:782:ALA:HB2	1.28	0.98
5:F:372:ARG:HG2	5:F:386:VAL:HG21	1.47	0.97
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.44	0.97
5:F:193:ARG:HB3	7:H:7:DC:H5"	1.52	0.92
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.07	0.88
5:F:371:LEU:O	5:F:381:HIS:ND1	2.07	0.88
1:B:38:ASN:HD21	2:C:979:THR:HG22	1.40	0.86
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.58	0.84
2:C:768:THR:OG1	2:C:771:GLU:OE1	1.97	0.82
1:A:206:THR:HG22	1:A:209:GLU:H	1.45	0.80
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.45	0.78
3:D:65:ARG:NH1	5:F:378:GLY:O	2.18	0.76
5:F:368:VAL:HG13	5:F:397:ILE:HG23	1.68	0.76
3:D:520:LEU:O	3:D:525:ARG:NH1	2.19	0.75
5:F:386:VAL:HB	5:F:397:ILE:HG21	1.68	0.75
3:D:960:LYS:NZ	3:D:1063:GLU:OE1	2.19	0.75
3:D:1126:ASP:O	3:D:1130:ARG:HA	1.86	0.75
5:F:365:GLU:OE2	5:F:403:LYS:NZ	2.20	0.75
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.69	0.74
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.19	0.74
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.69	0.74
2:C:55:GLU:O	2:C:56:GLU:HB2	1.87	0.74
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.69	0.74
2:C:602:GLU:HB2	2:C:648:ARG:HH11	1.52	0.74
3:D:65:ARG:HD3	5:F:378:GLY:O	1.87	0.73
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.22	0.73
5:F:419:ARG:HD3	5:F:422:LEU:HD12	1.71	0.73
5:F:383:LEU:HD21	5:F:398:ARG:HB2	1.70	0.72
5:F:372:ARG:NH1	5:F:381:HIS:O	2.22	0.72
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:769:PRO:HG3	3:D:65:ARG:NH1	2.05	0.71
1:A:185:ARG:HE	1:A:187:GLY:HA2	1.54	0.71
2:C:758:ARG:HH21	2:C:788:THR:HB	1.55	0.71
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.26	0.70
2:C:815:LEU:HD23	2:C:819:VAL:HG12	1.74	0.70
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.74	0.70
5:F:405:LEU:O	5:F:409:LYS:HG3	1.92	0.69
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.74	0.69
1:A:97:VAL:HG12	1:A:98:THR:H	1.56	0.68
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.75	0.68
2:C:249:LYS:HB3	2:C:252:LYS:HB2	1.76	0.68
3:D:500:ARG:NH1	3:D:1390:LEU:HD21	2.09	0.68
3:D:180:LYS:NZ	3:D:357:GLU:OE1	2.26	0.68
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.28	0.68
6:G:4:DT:H2"	6:G:5:DC:OP2	1.93	0.68
5:F:321:ILE:O	5:F:327:SER:OG	2.12	0.67
2:C:911:GLU:OE1	3:D:1062:ARG:NH1	2.27	0.67
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.77	0.67
1:B:112:ARG:NH1	1:B:126:ASP:OD1	2.28	0.67
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.75	0.67
2:C:118:ILE:HD11	2:C:382:ILE:HD13	1.75	0.67
1:A:206:THR:HG22	1:A:209:GLU:HG3	1.76	0.67
2:C:808:ARG:NH2	5:F:305:GLU:OE2	2.28	0.67
2:C:770:GLU:OE2	5:F:351:SER:OG	2.10	0.67
2:C:358:ARG:HB3	2:C:372:LEU:HD12	1.78	0.66
2:C:49:ARG:HB3	2:C:49:ARG:CZ	2.26	0.65
2:C:214:TYR:O	2:C:218:VAL:HG23	1.96	0.65
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.79	0.65
6:G:6:DC:N4	7:H:22:DG:O6	2.20	0.65
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.77	0.65
3:D:704:ARG:HB2	3:D:745:MET:HG2	1.77	0.65
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.12	0.64
2:C:711:GLU:OE2	2:C:816:LYS:NZ	2.27	0.64
2:C:853:LEU:HB2	2:C:858:MET:CE	2.27	0.64
3:D:1276:GLU:CD	3:D:1301:LYS:HZ3	2.01	0.64
2:C:937:ASP:OD1	2:C:939:ARG:HG2	1.98	0.64
5:F:392:VAL:HG21	5:F:396:ARG:HB2	1.78	0.64
3:D:711:LEU:HB3	3:D:714:GLN:HE21	1.63	0.64
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.31	0.64
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.79	0.64
2:C:168:ARG:NH1	2:C:345:ARG:HD3	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.33	0.64
2:C:49:ARG:HB3	2:C:49:ARG:NH1	2.13	0.63
3:D:45:PHE:O	3:D:86:ARG:NH2	2.31	0.63
2:C:571:LEU:CD2	2:C:700:TYR:HA	2.28	0.62
2:C:172:ILE:HD13	2:C:184:MET:HE3	1.81	0.62
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.31	0.62
2:C:271:GLU:OE1	2:C:288:ARG:NH1	2.33	0.62
3:D:1143:GLY:O	3:D:1147:ARG:HD2	1.99	0.62
2:C:428:ARG:NH2	2:C:447:ALA:O	2.33	0.61
2:C:230:ARG:HG3	2:C:233:GLU:HG3	1.83	0.61
3:D:1083:ASP:OD1	3:D:1238:MET:HB3	2.00	0.61
5:F:364:ARG:O	5:F:368:VAL:N	2.31	0.61
3:D:1277:ILE:HG13	3:D:1278:ASP:H	1.65	0.61
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.83	0.61
3:D:898:GLU:OE2	3:D:921:ARG:NH2	2.33	0.61
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.83	0.61
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.82	0.61
3:D:658:LEU:HD23	3:D:661:MET:HE1	1.83	0.61
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.83	0.60
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.82	0.60
3:D:234:GLU:HG3	3:D:234:GLU:O	2.00	0.60
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.83	0.60
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.82	0.60
2:C:221:LEU:HD11	2:C:307:LEU:HD21	1.82	0.60
1:A:89:PHE:HB2	1:A:146:ARG:NH2	2.16	0.60
2:C:587:VAL:O	2:C:591:SER:HB3	2.02	0.60
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.33	0.60
2:C:627:ARG:HD2	2:C:638:ASP:OD1	2.01	0.59
2:C:11:GLU:OE2	2:C:537:LYS:HE2	2.02	0.59
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.66	0.59
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.84	0.59
2:C:805:ARG:HG3	2:C:823:VAL:HG22	1.85	0.59
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.21	0.59
3:D:1283:ILE:HG12	3:D:1315:ASP:CG	2.23	0.58
3:D:56:TYR:HE1	3:D:69:GLU:HG3	1.67	0.58
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.85	0.58
2:C:771:GLU:HG3	2:C:775:ARG:HH22	1.68	0.58
5:F:398:ARG:O	5:F:402:ASN:ND2	2.30	0.58
3:D:97:THR:OG1	3:D:571:LYS:HE2	2.04	0.58
3:D:231:VAL:O	3:D:236:TYR:OH	2.20	0.58
3:D:1087:ARG:HG3	3:D:1256:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:372:ARG:CZ	5:F:372:ARG:HB3	2.25	0.58
1:A:186:LEU:HB3	1:A:188:GLN:OE1	2.04	0.58
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.39	0.58
1:B:18:ARG:O	1:B:207:PRO:HD3	2.02	0.58
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.68	0.58
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.86	0.58
3:D:907:GLU:HB2	3:D:1026:SER:HA	1.86	0.58
5:F:368:VAL:HG11	5:F:400:ILE:HG13	1.84	0.58
1:A:58:ILE:HG21	1:A:68:ILE:HD11	1.86	0.57
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.39	0.57
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.85	0.57
1:A:103:ALA:HB1	1:A:107:LYS:HE3	1.86	0.57
2:C:421:GLU:HB2	6:G:13:DA:C2	2.39	0.57
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.85	0.57
3:D:1284:GLU:HG2	3:D:1291:SER:HB3	1.87	0.57
5:F:321:ILE:HG22	6:G:19:DC:H2"	1.86	0.57
3:D:860:LEU:O	3:D:876:SER:HB2	2.03	0.57
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.40	0.57
1:B:80:LEU:HD22	3:D:844:ALA:HA	1.85	0.56
2:C:573:ARG:HB2	2:C:670:GLN:HE22	1.70	0.56
3:D:1459:LEU:HD23	3:D:1464:GLU:HB3	1.87	0.56
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.05	0.56
1:A:70:GLY:N	2:C:607:ASP:OD1	2.35	0.56
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.87	0.56
5:F:202:TYR:HE2	5:F:248:ASN:HD21	1.51	0.56
5:F:82:ARG:HB2	7:H:8:DG:O6	2.05	0.56
3:D:1450:ALA:HA	3:D:1455:LYS:HD2	1.86	0.56
2:C:413:LEU:HD21	2:C:451:LEU:HD13	1.88	0.56
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.88	0.56
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.39	0.56
3:D:1152:GLU:OE1	3:D:1159:ARG:NH1	2.39	0.56
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.86	0.56
2:C:167:LYS:HD3	7:H:12:DT:H72	1.88	0.55
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.88	0.55
1:A:201:THR:HG21	1:A:205:VAL:O	2.06	0.55
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.88	0.55
1:B:49:PRO:HA	1:B:148:VAL:HG12	1.89	0.55
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.88	0.55
3:D:475:LYS:O	3:D:479:GLU:HG2	2.07	0.55
3:D:514:LEU:HD13	3:D:517:VAL:HG22	1.89	0.55
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:750:PRO:O	3:D:756:GLN:NE2	2.40	0.55
3:D:922:LEU:HB3	3:D:926:LYS:HD2	1.87	0.55
2:C:513:VAL:HG22	2:C:524:VAL:HG12	1.88	0.54
3:D:181:ASP:HB2	3:D:205:TYR:CG	2.42	0.54
5:F:369:LEU:HD13	5:F:401:GLU:HG3	1.88	0.54
2:C:395:LYS:HE2	2:C:403:SER:HB2	1.89	0.54
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.88	0.54
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.35	0.54
3:D:1272:ALA:HA	3:D:1326:THR:HB	1.89	0.54
3:D:322:VAL:HG22	3:D:335:LEU:CD2	2.38	0.54
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.90	0.54
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.89	0.54
1:B:56:VAL:HG23	1:B:142:VAL:HG12	1.89	0.54
2:C:567:GLN:HB2	2:C:997:LEU:HD22	1.88	0.54
2:C:767:PRO:HB2	2:C:771:GLU:HB3	1.89	0.54
3:D:351:MET:HG2	3:D:370:ALA:HB2	1.90	0.54
2:C:595:LEU:HD21	2:C:623:TYR:HB3	1.89	0.54
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.89	0.54
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.90	0.53
2:C:614:ARG:NH2	2:C:618:GLY:O	2.38	0.53
3:D:248:PRO:HG3	3:D:308:LYS:HG3	1.89	0.53
1:A:191:ASP:OD1	2:C:938:LYS:NZ	2.41	0.53
3:D:288:MET:HG2	3:D:307:ALA:HB2	1.91	0.53
3:D:1276:GLU:OE2	3:D:1301:LYS:NZ	2.40	0.53
3:D:134:VAL:HG23	3:D:149:LYS:HA	1.91	0.53
1:A:97:VAL:HG12	1:A:98:THR:N	2.22	0.53
1:B:216:GLU:CD	1:B:219:ARG:HH21	2.11	0.53
3:D:892:ASP:OD1	3:D:894:LYS:HD2	2.09	0.53
1:A:89:PHE:HB2	1:A:146:ARG:HH22	1.73	0.53
3:D:1049:SER:OG	3:D:1051:GLU:HG2	2.09	0.53
3:D:658:LEU:HD23	3:D:661:MET:CE	2.38	0.53
3:D:489:ARG:NH1	3:D:1391:GLU:OE2	2.42	0.53
3:D:114:THR:HG23	3:D:495:ARG:HG2	1.91	0.53
5:F:383:LEU:CD2	5:F:398:ARG:HB2	2.39	0.53
2:C:722:ILE:HD12	2:C:821:GLU:HG3	1.91	0.52
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.43	0.52
2:C:1023:GLY:HA2	6:G:18:DC:OP2	2.09	0.52
2:C:838:LYS:HE3	3:D:741:ASP:O	2.10	0.52
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.39	0.52
2:C:750:LYS:HD2	3:D:681:ARG:HE	1.74	0.52
2:C:239:PHE:CD2	2:C:253:ALA:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.92	0.52
2:C:875:GLY:O	2:C:879:ARG:HD3	2.09	0.52
1:B:38:ASN:ND2	2:C:979:THR:HG22	2.19	0.52
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.45	0.52
3:D:134:VAL:HG22	3:D:151:GLN:H	1.74	0.52
1:B:80:LEU:HD22	3:D:844:ALA:CA	2.40	0.52
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.43	0.51
3:D:59:ALA:HB2	3:D:78:VAL:HG21	1.93	0.51
3:D:683:ILE:HG23	3:D:687:VAL:HG21	1.92	0.51
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.31	0.51
2:C:807:ARG:HG2	2:C:821:GLU:HB3	1.91	0.51
2:C:858:MET:HG2	2:C:867:VAL:O	2.09	0.51
3:D:640:HIS:CD2	3:D:641:GLN:HG3	2.45	0.51
2:C:1006:HIS:HB2	2:C:1024:LYS:HG3	1.92	0.51
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.93	0.51
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.91	0.51
1:A:57:TYR:CD1	1:A:161:ARG:HD2	2.46	0.51
3:D:1281:VAL:HG23	3:D:1317:ASP:O	2.10	0.51
3:D:202:VAL:HG21	3:D:400:VAL:HG13	1.93	0.51
2:C:171:TRP:CH2	7:H:12:DT:H2"	2.46	0.51
2:C:470:PRO:HD3	2:C:485:TYR:CE2	2.46	0.51
3:D:1031:ASN:O	3:D:1035:ILE:HG12	2.10	0.51
5:F:376:ILE:HG22	5:F:377:ASP:OD2	2.10	0.51
2:C:1103:ASP:OD2	2:C:1107:ASN:HB2	2.11	0.51
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	2.26	0.51
5:F:367:MET:HG3	5:F:390:PHE:HZ	1.76	0.51
2:C:374:ASN:OD1	5:F:276:ARG:HD2	2.11	0.51
2:C:272:ALA:HA	2:C:464:LEU:HD13	1.92	0.51
5:F:130:VAL:HG21	5:F:159:ILE:HG21	1.92	0.51
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.45	0.50
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	1.93	0.50
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.46	0.50
5:F:193:ARG:HB3	7:H:7:DC:C5'	2.33	0.50
5:F:193:ARG:NH1	7:H:7:DC:H5	2.09	0.50
5:F:202:TYR:HE2	5:F:248:ASN:ND2	2.09	0.50
5:F:396:ARG:HG2	5:F:399:GLN:NE2	2.26	0.50
2:C:211:LEU:HD23	2:C:311:PHE:CD2	2.46	0.50
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.46	0.50
3:D:564:GLU:OE2	5:F:140:ARG:NH2	2.43	0.50
2:C:563:ASN:O	2:C:566:THR:HB	2.11	0.50
3:D:131:LYS:O	3:D:456:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:483:HIS:CE1	3:D:488:ARG:HG3	2.46	0.50
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.93	0.50
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.47	0.50
3:D:675:ARG:HH11	3:D:675:ARG:CB	2.25	0.50
5:F:141:VAL:HG21	5:F:153:PRO:HD3	1.94	0.50
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.41	0.49
2:C:757:GLY:HA2	2:C:789:SER:OG	2.11	0.49
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.46	0.49
1:B:38:ASN:HB3	1:B:39:PRO:HD3	1.93	0.49
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.95	0.49
2:C:154:ARG:HH12	2:C:178:PRO:HB3	1.76	0.49
2:C:740:GLU:HB3	2:C:805:ARG:HH12	1.77	0.49
2:C:194:VAL:HG22	2:C:221:LEU:HD23	1.93	0.49
3:D:1271:LYS:HG3	3:D:1272:ALA:O	2.13	0.49
3:D:502:PHE:HD2	3:D:507:ASN:O	1.95	0.49
3:D:899:LEU:HD22	3:D:917:GLN:HB3	1.93	0.49
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.12	0.49
3:D:201:GLY:HA3	3:D:396:VAL:O	2.13	0.49
2:C:312:ALA:HB1	2:C:317:VAL:HB	1.94	0.49
2:C:50:GLU:OE1	2:C:345:ARG:NE	2.44	0.49
3:D:155:ASP:OD1	3:D:568:ARG:NH1	2.44	0.49
3:D:238:PRO:CD	3:D:318:ARG:HG3	2.36	0.49
5:F:154:LYS:O	5:F:158:GLU:HG3	2.13	0.49
2:C:436:GLY:HA2	2:C:538:GLN:O	2.13	0.49
2:C:472:ARG:HD2	2:C:480:THR:O	2.11	0.49
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.94	0.49
3:D:1290:LEU:HD12	3:D:1291:SER:H	1.78	0.49
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.47	0.49
2:C:1053:LEU:HA	3:D:621:LYS:HD2	1.95	0.49
6:G:3:DC:H2"	6:G:4:DT:H5'	1.94	0.49
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.95	0.48
2:C:815:LEU:HD23	2:C:819:VAL:CG1	2.42	0.48
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.94	0.48
5:F:392:VAL:CG1	5:F:396:ARG:HD2	2.44	0.48
1:A:94:LEU:O	1:A:146:ARG:NH1	2.47	0.48
2:C:573:ARG:HB2	2:C:670:GLN:NE2	2.27	0.48
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.47	0.48
3:D:298:VAL:HA	3:D:302:GLN:OE1	2.13	0.48
3:D:307:ALA:HB1	3:D:311:LEU:HD23	1.95	0.48
3:D:405:ASP:CG	3:D:406:ASP:H	2.17	0.48
3:D:806:PHE:O	3:D:829:VAL:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:VAL:HG11	2:C:472:ARG:HD3	1.95	0.48
2:C:470:PRO:HD3	2:C:485:TYR:HE2	1.77	0.48
3:D:214:GLU:HB3	3:D:340:THR:HB	1.95	0.48
3:D:636:GLN:NE2	3:D:637:LEU:HG	2.29	0.48
2:C:118:ILE:CD1	2:C:382:ILE:HD13	2.43	0.48
3:D:322:VAL:HG22	3:D:335:LEU:HD21	1.96	0.48
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.96	0.48
5:F:96:LEU:O	5:F:100:VAL:HG23	2.14	0.48
2:C:1035:MET:HA	2:C:1038:TRP:CE3	2.49	0.48
3:D:841:TYR:HB2	3:D:864:VAL:HG22	1.95	0.48
5:F:188:ILE:HG12	5:F:224:VAL:HG21	1.94	0.48
1:B:161:ARG:HG3	1:B:162:ILE:O	2.14	0.48
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.96	0.48
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.49	0.48
3:D:258:VAL:HG12	3:D:273:ARG:O	2.13	0.48
5:F:361:LEU:HD13	5:F:365:GLU:HG3	1.96	0.48
1:B:179:PHE:HB3	1:B:197:LEU:HD12	1.96	0.47
2:C:926:PHE:CZ	2:C:930:LYS:HD3	2.49	0.47
1:B:101:LEU:HD11	1:B:113:ASP:HB2	1.96	0.47
1:A:30:ARG:HH22	3:D:855:HIS:HD2	1.61	0.47
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.13	0.47
1:A:74:ASP:OD1	1:A:76:VAL:HB	2.14	0.47
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.96	0.47
3:D:1450:ALA:HA	3:D:1455:LYS:CD	2.44	0.47
5:F:188:ILE:HD13	5:F:221:ILE:HG12	1.96	0.47
5:F:237:THR:OG1	7:H:4:DA:H2'	2.15	0.47
3:D:1444:THR:O	3:D:1448:THR:HG23	2.14	0.47
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.49	0.47
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.96	0.47
5:F:193:ARG:NH1	7:H:7:DC:C5	2.83	0.47
3:D:242:LEU:HD23	3:D:285:PRO:HG3	1.97	0.47
5:F:355:GLU:OE2	5:F:370:LYS:NZ	2.42	0.47
5:F:194:LEU:HB2	7:H:6:DT:C2	2.50	0.47
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.97	0.47
2:C:910:LYS:O	2:C:914:ILE:HG13	2.15	0.47
6:G:17:DT:H71	6:G:18:DC:N4	2.30	0.47
2:C:1:MET:HB2	2:C:898:GLY:O	2.15	0.46
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.96	0.46
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.97	0.46
6:G:3:DC:H2'	6:G:4:DT:H72	1.97	0.46
2:C:243:ARG:HH21	7:H:9:DA:N6	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:69:LEU:HD23	2:C:69:LEU:HA	1.78	0.46
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.96	0.46
2:C:206:THR:O	2:C:210:GLU:HB2	2.14	0.46
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.96	0.46
2:C:56:GLU:HG3	2:C:359:MET:HE3	1.98	0.46
2:C:591:SER:O	2:C:592:LEU:HB2	2.15	0.46
2:C:548:PRO:O	2:C:843:HIS:HE1	1.98	0.46
4:E:46:PRO:HD2	4:E:63:TRP:CE2	2.50	0.46
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.97	0.46
5:F:368:VAL:HG21	5:F:400:ILE:CD1	2.45	0.46
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.43	0.46
5:F:357:ALA:HB1	5:F:408:LEU:HD22	1.97	0.46
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.96	0.46
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.50	0.46
3:D:67:ARG:HH11	5:F:379:ARG:HD3	1.81	0.46
1:A:6:LEU:HD23	1:A:189:ARG:CZ	2.46	0.46
1:A:206:THR:CG2	1:A:209:GLU:HG3	2.44	0.46
2:C:775:ARG:NE	2:C:782:ALA:HB2	2.12	0.46
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.97	0.46
3:D:879:ARG:HB3	3:D:902:LEU:CD1	2.45	0.46
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.76	0.46
3:D:480:GLU:OE2	3:D:488:ARG:HD2	2.15	0.46
1:B:73:GLU:N	1:B:73:GLU:OE1	2.37	0.46
3:D:236:TYR:CE1	3:D:242:LEU:HA	2.51	0.46
3:D:711:LEU:HD13	3:D:778:LEU:HD13	1.97	0.46
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.98	0.45
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.51	0.45
2:C:1070:ILE:CG2	3:D:655:PRO:HB2	2.45	0.45
2:C:164:PRO:HA	2:C:269:LEU:HD12	1.99	0.45
2:C:617:ASP:OD1	2:C:617:ASP:N	2.49	0.45
3:D:1277:ILE:HG13	3:D:1278:ASP:N	2.31	0.45
2:C:425:PHE:CD1	3:D:1079:LYS:HE3	2.51	0.45
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.19	0.45
3:D:949:ILE:HD11	3:D:1023:MET:CE	2.47	0.45
5:F:127:ILE:O	5:F:131:VAL:HG23	2.17	0.45
6:G:8:DG:H2"	6:G:9:DG:C8	2.52	0.45
1:A:226:SER:O	1:A:228:PRO:HD3	2.16	0.45
3:D:215:TYR:O	3:D:340:THR:HA	2.15	0.45
3:D:1211:MET:SD	4:E:16:LYS:HE2	2.56	0.45
6:G:15:DT:H2'	6:G:16:DG:C8	2.51	0.45
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:TYR:CE1	2:C:304:LEU:HD22	2.51	0.45
2:C:708:TYR:HB3	2:C:790:LEU:HD21	1.98	0.45
3:D:1047:LYS:HG2	3:D:1053:PHE:CE1	2.52	0.45
3:D:1125:PRO:HB2	3:D:1130:ARG:HH22	1.81	0.45
3:D:1198:TYR:CE1	3:D:1460:ILE:HD13	2.51	0.45
3:D:452:ILE:HD13	3:D:452:ILE:HG21	1.73	0.45
5:F:421:PHE:N	5:F:421:PHE:CD2	2.85	0.45
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.52	0.45
3:D:1087:ARG:HG3	3:D:1256:LEU:CD2	2.46	0.45
3:D:645:PRO:HB3	3:D:723:GLY:O	2.16	0.45
2:C:424:GLY:O	2:C:427:VAL:HG23	2.17	0.45
3:D:1383:ASP:OD2	3:D:1385:GLY:N	2.48	0.45
3:D:417:PRO:HB3	3:D:430:ASP:O	2.17	0.45
2:C:293:PHE:HD1	2:C:298:PHE:CE2	2.34	0.45
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.32	0.45
3:D:465:LEU:HA	3:D:465:LEU:HD23	1.72	0.45
1:B:65:PHE:CD2	3:D:809:PRO:HB2	2.51	0.45
2:C:312:ALA:HB3	2:C:320:HIS:CD2	2.52	0.44
2:C:56:GLU:HG3	2:C:359:MET:CE	2.47	0.44
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.82	0.44
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.52	0.44
2:C:267:TYR:CE2	2:C:290:LEU:HG	2.52	0.44
3:D:1445:HIS:HE1	3:D:1449:GLU:OE1	2.00	0.44
3:D:661:MET:HE2	3:D:677:LEU:HD11	1.99	0.44
3:D:876:SER:OG	3:D:879:ARG:HG3	2.17	0.44
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.99	0.44
1:A:201:THR:HG22	1:A:202:ASP:N	2.32	0.44
2:C:425:PHE:HD1	3:D:1079:LYS:HE3	1.82	0.44
3:D:44:LEU:O	3:D:525:ARG:NH2	2.50	0.44
3:D:536:ALA:HA	5:F:315:VAL:O	2.17	0.44
3:D:654:LYS:HB3	3:D:655:PRO:HD3	1.99	0.44
3:D:129:PHE:CZ	3:D:571:LYS:HB3	2.53	0.44
3:D:632:VAL:O	3:D:727:GLN:HA	2.17	0.44
4:E:46:PRO:HB2	4:E:57:ASP:CB	2.47	0.44
2:C:118:ILE:HD12	2:C:118:ILE:HG23	1.79	0.44
2:C:473:ARG:HG3	2:C:474:VAL:N	2.33	0.44
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	2.00	0.44
3:D:657:LEU:HG	3:D:661:MET:HE2	1.99	0.44
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.52	0.44
1:A:32:PHE:HA	1:A:35:THR:HB	2.00	0.44
2:C:592:LEU:HD23	2:C:592:LEU:HA	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:166:LEU:HA	5:F:166:LEU:HD23	1.84	0.44
5:F:365:GLU:HA	5:F:368:VAL:HB	2.00	0.44
2:C:170:PRO:HD2	2:C:267:TYR:CE1	2.53	0.44
2:C:194:VAL:HG13	2:C:221:LEU:HD23	1.99	0.44
3:D:1000:THR:HG23	3:D:1036:ARG:HD2	1.99	0.44
3:D:1405:GLU:HA	3:D:1408:ILE:HG22	2.00	0.44
2:C:557:ARG:HG3	2:C:844:GLY:HA3	2.00	0.44
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.51	0.44
2:C:1060:ILE:HD11	2:C:1083:GLU:HG2	1.99	0.43
2:C:797:GLY:O	2:C:829:GLN:NE2	2.51	0.43
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.99	0.43
3:D:1493:LYS:HA	3:D:1496:GLU:OE1	2.18	0.43
3:D:357:GLU:HB2	3:D:387:LEU:HD23	1.99	0.43
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.63	0.43
2:C:683:ASN:HB3	2:C:872:ASN:HB2	2.00	0.43
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.51	0.43
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.53	0.43
3:D:703:ASN:HA	3:D:712:GLY:O	2.18	0.43
5:F:81:VAL:HG23	5:F:210:LEU:HD11	2.00	0.43
2:C:468:ARG:HA	2:C:486:MET:O	2.17	0.43
3:D:1459:LEU:CD2	3:D:1464:GLU:HB3	2.48	0.43
2:C:136:ILE:HB	2:C:336:VAL:HG13	2.00	0.43
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.65	0.43
3:D:17:LYS:HB2	3:D:17:LYS:HE2	1.74	0.43
5:F:324:GLU:HB2	5:F:326:ASP:OD1	2.19	0.43
5:F:198:ILE:HD12	5:F:243:ILE:HG21	1.99	0.43
1:B:111:ALA:HB3	1:B:125:PRO:HA	2.01	0.43
2:C:678:PRO:HA	2:C:683:ASN:HD22	1.82	0.43
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.99	0.43
2:C:772:ARG:NE	5:F:380:GLU:OE1	2.52	0.43
1:A:106:PRO:CG	1:A:134:GLU:HG2	2.48	0.43
1:A:6:LEU:HD23	1:A:189:ARG:NH2	2.33	0.43
1:B:65:PHE:HD2	3:D:809:PRO:HB2	1.83	0.43
2:C:170:PRO:HD2	2:C:267:TYR:HE1	1.83	0.43
2:C:133:ASP:HB3	2:C:395:LYS:HD2	2.01	0.43
3:D:56:TYR:CE1	3:D:69:GLU:HG3	2.51	0.43
5:F:408:LEU:HD23	5:F:408:LEU:HA	1.67	0.43
1:A:80:LEU:HA	1:A:80:LEU:HD12	1.88	0.43
2:C:879:ARG:HD2	2:C:879:ARG:N	2.34	0.43
3:D:123:LEU:HA	3:D:123:LEU:HD12	1.72	0.43
5:F:130:VAL:HG11	5:F:159:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:415:THR:HB	5:F:417:LYS:HE3	2.01	0.43
1:B:85:LEU:HG	1:B:87:VAL:HG23	2.01	0.43
2:C:12:VAL:HG21	2:C:472:ARG:HD3	2.00	0.43
2:C:376:ARG:HB2	2:C:377:PRO:HD3	2.01	0.43
3:D:1232:PRO:O	3:D:1235:GLN:HB2	2.18	0.43
3:D:1339:LYS:HB3	3:D:1343:ALA:HB3	2.01	0.43
3:D:684:LYS:HB3	3:D:684:LYS:HE2	1.55	0.43
5:F:321:ILE:CG2	6:G:19:DC:H2"	2.49	0.43
2:C:260:LEU:O	2:C:261:ILE:HD12	2.19	0.42
3:D:1127:GLU:HA	3:D:1130:ARG:HE	1.84	0.42
3:D:103:TRP:HB3	3:D:1448:THR:HG21	2.00	0.42
3:D:399:ARG:HB2	3:D:401:TYR:CE1	2.53	0.42
5:F:163:LEU:HD13	5:F:174:LEU:HD13	2.01	0.42
3:D:1014:ASN:OD1	3:D:1014:ASN:N	2.52	0.42
3:D:15:PRO:O	3:D:19:ARG:HG3	2.18	0.42
3:D:573:MET:SD	5:F:210:LEU:HB3	2.59	0.42
3:D:1486:VAL:HG22	4:E:22:VAL:HG13	2.02	0.42
3:D:351:MET:HE1	3:D:375:GLU:O	2.19	0.42
3:D:613:ARG:HG3	3:D:618:LEU:HD23	2.01	0.42
3:D:1495:ILE:HG12	4:E:88:GLU:CG	2.49	0.42
7:H:8:DG:C5	7:H:9:DA:C6	3.08	0.42
2:C:214:TYR:HB3	2:C:217:LEU:HD12	2.00	0.42
3:D:1052:THR:HG22	3:D:1053:PHE:O	2.19	0.42
5:F:358:LEU:HA	5:F:358:LEU:HD23	1.83	0.42
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.85	0.42
2:C:545:ASN:HB3	2:C:583:LEU:HD22	2.01	0.42
2:C:638:ASP:OD2	2:C:640:ARG:HD2	2.19	0.42
2:C:862:PRO:HA	2:C:975:TYR:CE2	2.55	0.42
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.84	0.42
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.74	0.42
2:C:81:ASP:OD1	2:C:81:ASP:N	2.43	0.42
2:C:905:ILE:C	2:C:907:ASP:H	2.23	0.42
2:C:679:PHE:HA	3:D:943:THR:HG23	2.00	0.42
2:C:886:LEU:HD21	3:D:951:ILE:HG12	2.00	0.42
1:B:110:LYS:HD2	1:B:128:HIS:HA	2.02	0.42
2:C:118:ILE:HA	2:C:118:ILE:HD13	1.69	0.42
2:C:32:ALA:HB2	2:C:73:LEU:HD12	2.02	0.42
2:C:755:LEU:HA	2:C:755:LEU:HD23	1.81	0.42
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.77	0.42
5:F:367:MET:CG	5:F:390:PHE:HZ	2.33	0.42
2:C:884:GLN:HB2	2:C:992:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1276:GLU:CD	3:D:1301:LYS:NZ	2.72	0.42
3:D:134:VAL:CG2	3:D:151:GLN:H	2.33	0.42
3:D:156:GLU:H	3:D:156:GLU:CD	2.23	0.42
3:D:236:TYR:HB3	3:D:313:MET:HG3	2.00	0.42
3:D:654:LYS:O	3:D:658:LEU:HG	2.18	0.42
7:H:7:DC:H5'	7:H:7:DC:H6	1.84	0.42
1:A:47:SER:O	1:A:49:PRO:HD3	2.20	0.42
2:C:127:PHE:O	2:C:133:ASP:HA	2.19	0.42
2:C:179:ASN:OD1	2:C:181:VAL:HG12	2.19	0.42
2:C:261:ILE:HG22	2:C:262:ALA:N	2.34	0.42
2:C:657:ASP:OD2	2:C:663:ASN:N	2.48	0.42
3:D:949:ILE:HD11	3:D:1023:MET:HE1	2.02	0.42
3:D:1068:LEU:HD12	3:D:1068:LEU:HA	1.85	0.42
3:D:1236:LEU:HA	3:D:1359:GLN:HG3	2.01	0.42
2:C:168:ARG:O	2:C:267:TYR:HA	2.19	0.41
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.80	0.41
2:C:344:PHE:CD2	2:C:382:ILE:HD11	2.54	0.41
3:D:1144:LEU:HD23	3:D:1144:LEU:HA	1.73	0.41
2:C:682:TYR:CE1	3:D:635:PRO:HD2	2.55	0.41
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.54	0.41
2:C:580:MET:HB3	2:C:584:GLU:CD	2.41	0.41
2:C:767:PRO:HB2	2:C:771:GLU:CB	2.50	0.41
3:D:1377:LYS:HE3	3:D:1378:TYR:OH	2.19	0.41
3:D:842:VAL:HG22	3:D:865:THR:HB	2.01	0.41
3:D:879:ARG:HB3	3:D:902:LEU:HD11	2.02	0.41
3:D:970:LYS:HD2	3:D:970:LYS:HA	1.93	0.41
1:B:7:LYS:HB2	1:B:7:LYS:HE3	1.88	0.41
3:D:1359:GLN:HA	3:D:1359:GLN:NE2	2.35	0.41
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.34	0.41
3:D:625:TYR:CE1	3:D:751:LEU:HD11	2.55	0.41
1:B:38:ASN:HD21	2:C:979:THR:CG2	2.22	0.41
2:C:99:GLN:OE1	2:C:101:ILE:HD11	2.20	0.41
2:C:598:GLU:O	2:C:651:LYS:HG3	2.21	0.41
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.82	0.41
3:D:687:VAL:O	3:D:690:ALA:HB3	2.20	0.41
2:C:770:GLU:HB3	5:F:350:LEU:CD2	2.50	0.41
2:C:874:LEU:HA	2:C:874:LEU:HD23	1.89	0.41
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.55	0.41
2:C:269:LEU:HA	2:C:269:LEU:HD12	1.92	0.41
2:C:675:ALA:HB2	2:C:867:VAL:HG11	2.03	0.41
2:C:807:ARG:HG2	2:C:821:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:115:LYS:HG2	5:F:173:TYR:CE1	2.55	0.41
3:D:1140:ILE:CG2	3:D:1144:LEU:HD12	2.51	0.41
3:D:704:ARG:HB2	3:D:745:MET:HE2	2.03	0.41
3:D:75:ARG:HB2	3:D:75:ARG:HE	1.73	0.41
4:E:36:LYS:CG	4:E:93:TYR:HB3	2.51	0.41
1:A:20:TYR:C	1:A:207:PRO:HG2	2.41	0.41
2:C:99:GLN:O	2:C:99:GLN:HG3	2.21	0.41
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.54	0.41
3:D:547:LEU:HD12	3:D:547:LEU:HA	1.77	0.41
3:D:57:GLU:OE2	3:D:64:LYS:HE2	2.21	0.41
2:C:593:ALA:HB1	2:C:659:PRO:HD2	2.02	0.41
2:C:899:GLN:HG3	2:C:901:TYR:CZ	2.55	0.41
1:B:13:VAL:HG13	1:B:23:PHE:CE1	2.56	0.41
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.86	0.41
3:D:1125:PRO:HA	3:D:1132:LEU:HD23	2.03	0.41
3:D:501:ALA:HB1	3:D:1452:ILE:HG22	2.02	0.41
3:D:185:VAL:HG13	3:D:189:GLN:HB3	2.02	0.41
5:F:412:GLU:OE1	5:F:418:LEU:HB2	2.21	0.41
2:C:767:PRO:CB	2:C:771:GLU:HB3	2.50	0.41
3:D:12:LEU:HA	3:D:12:LEU:HD23	1.78	0.41
3:D:1381:VAL:HG21	3:D:1389:LEU:HD23	2.03	0.41
3:D:366:LYS:HE3	3:D:366:LYS:HB2	1.83	0.41
3:D:41:ARG:NH1	3:D:48:ARG:NH1	2.69	0.41
3:D:625:TYR:CD1	3:D:751:LEU:HD11	2.56	0.41
5:F:354:LEU:HD23	5:F:354:LEU:HA	1.94	0.41
2:C:740:GLU:HB3	2:C:805:ARG:NH1	2.36	0.40
3:D:709:HIS:HA	3:D:1227:GLN:HB3	2.03	0.40
3:D:792:ILE:HG13	3:D:793:THR:HG23	2.02	0.40
3:D:834:THR:OG1	3:D:838:ARG:HD2	2.21	0.40
6:G:4:DT:C2'	6:G:5:DC:OP2	2.65	0.40
2:C:304:LEU:HB3	2:C:305:PRO:HD3	2.03	0.40
3:D:432:TYR:O	3:D:448:GLU:HA	2.21	0.40
3:D:67:ARG:HB3	5:F:377:ASP:O	2.22	0.40
5:F:392:VAL:CG2	5:F:396:ARG:HB2	2.49	0.40
3:D:1372:VAL:HA	3:D:1375:MET:HE3	2.04	0.40
3:D:288:MET:HA	3:D:306:GLU:O	2.20	0.40
3:D:695:ILE:HD12	3:D:718:PRO:HG2	2.04	0.40
3:D:853:VAL:HG22	3:D:858:VAL:HG23	2.03	0.40
2:C:154:ARG:NH1	2:C:178:PRO:HB3	2.37	0.40
2:C:501:THR:HA	2:C:502:PRO:HD3	1.97	0.40
5:F:101:GLU:HG2	5:F:105:LYS:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:392:VAL:CG2	5:F:397:ILE:HG12	2.51	0.40
1:A:71:VAL:HG22	1:A:132:LEU:HG	2.02	0.40
2:C:136:ILE:HD13	2:C:392:SER:HA	2.03	0.40
2:C:710:ILE:HD12	2:C:790:LEU:HB2	2.03	0.40
2:C:987:ILE:HD11	3:D:946:GLY:HA2	2.03	0.40
3:D:629:SER:OG	3:D:630:VAL:N	2.54	0.40
5:F:345:ALA:O	5:F:349:LEU:HG	2.22	0.40
5:F:396:ARG:HA	5:F:399:GLN:HG2	2.01	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)
2:C:68:PHE:O	5:F:396:ARG:NH2[1_545]	1.84	0.36

5.3 Torsion angles

5.3.1 Protein backbone

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%)	222 (99%)	2 (1%)	0	100	100
1	B	220/315 (70%)	209 (95%)	10 (4%)	1 (0%)	29	60
2	C	1107/1119 (99%)	1077 (97%)	27 (2%)	3 (0%)	41	70
3	D	1482/1524 (97%)	1444 (97%)	35 (2%)	3 (0%)	47	77
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	14	42
5	F	344/423 (81%)	327 (95%)	14 (4%)	3 (1%)	17	47
All	All	3469/3795 (91%)	3368 (97%)	90 (3%)	11 (0%)	41	70

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	1130	ARG
1	B	154	GLU
2	C	764	GLU
3	D	1236	LEU
5	F	356	LYS
2	C	105	THR
5	F	384	GLU
3	D	320	ALA
5	F	148	LYS
4	E	94	PRO
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%)	192 (96%)	7 (4%)	36	66
1	B	195/273 (71%)	190 (97%)	5 (3%)	46	72
2	C	935/941 (99%)	891 (95%)	44 (5%)	26	56
3	D	1253/1279 (98%)	1187 (95%)	66 (5%)	22	51
4	E	83/88 (94%)	81 (98%)	2 (2%)	49	74
5	F	301/371 (81%)	294 (98%)	7 (2%)	50	75
All	All	2966/3225 (92%)	2835 (96%)	131 (4%)	28	58

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	133	GLU
1	A	184	THR
1	A	189	ARG
1	A	206	THR
1	A	229	GLN
1	B	7	LYS

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Mol	Chain	Res	Type
1	B	29	GLU
1	B	34	VAL
1	B	186	LEU
1	B	190	THR
2	C	8	ARG
2	C	15	LEU
2	C	81	ASP
2	C	107	LEU
2	C	133	ASP
2	C	141	HIS
2	C	168	ARG
2	C	205	GLU
2	C	221	LEU
2	C	251	ASP
2	C	284	ARG
2	C	342	ASP
2	C	353	ARG
2	C	358	ARG
2	C	409	ARG
2	C	427	VAL
2	C	434	HIS
2	C	449	ILE
2	C	454	SER
2	C	460	ARG
2	C	480	THR
2	C	524	VAL
2	C	557	ARG
2	C	575	GLN
2	C	583	LEU
2	C	586	ARG
2	C	589	ARG
2	C	591	SER
2	C	610	ARG
2	C	617	ASP
2	C	640	ARG
2	C	661	SER
2	C	715	THR
2	C	764	GLU
2	C	775	ARG
2	C	808	ARG
2	C	815	LEU
2	C	939	ARG

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Mol	Chain	Res	Type
2	C	942	GLU
2	C	948	GLU
2	C	968	LEU
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
3	D	30	GLU
3	D	67	ARG
3	D	68	PHE
3	D	81	THR
3	D	106	LYS
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	200	ASP
3	D	204	LEU
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	276	ASP
3	D	312	ARG
3	D	325	GLU
3	D	362	GLU
3	D	372	ASP
3	D	411	THR
3	D	421	LEU
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	675	ARG
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	808	THR
3	D	817	GLU

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Mol	Chain	Res	Type
3	D	832	ARG
3	D	834	THR
3	D	864	VAL
3	D	875	THR
3	D	894	LYS
3	D	904	VAL
3	D	970	LYS
3	D	972	LEU
3	D	1014	ASN
3	D	1041	LEU
3	D	1062	ARG
3	D	1067	VAL
3	D	1119	SER
3	D	1130	ARG
3	D	1155	VAL
3	D	1182	GLU
3	D	1188	VAL
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1271	LYS
3	D	1282	ARG
3	D	1284	GLU
3	D	1288	GLU
3	D	1290	LEU
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP
3	D	1455	LYS
3	D	1470	ARG
4	E	50	THR
4	E	89	MET
5	F	159	ILE
5	F	172	ARG
5	F	186	HIS
5	F	205	ARG
5	F	348	SER
5	F	372	ARG
5	F	421	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	ASN
2	C	565	GLN
2	C	683	ASN
2	C	834	GLN
3	D	636	GLN
3	D	714	GLN
3	D	724	GLN
3	D	994	GLN
3	D	1359	GLN
3	D	1445	HIS
5	F	248	ASN
5	F	269	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.29	0	100	100	70, 93, 114, 122	0
1	B	222/315 (70%)	-0.32	0	100	100	68, 96, 123, 140	0
2	C	1111/1119 (99%)	-0.08	34 (3%)	49	25	53, 93, 163, 194	0
3	D	1486/1524 (97%)	-0.18	24 (1%)	72	49	49, 87, 150, 181	0
4	E	94/99 (94%)	-0.27	0	100	100	66, 95, 132, 147	0
5	F	346/423 (81%)	0.47	49 (14%)	2	1	62, 107, 194, 203	0
6	G	18/21 (85%)	0.01	1 (5%)	24	10	98, 119, 167, 170	0
7	H	22/27 (81%)	-0.32	2 (9%)	9	3	88, 126, 166, 182	0
All	All	3525/3843 (91%)	-0.10	110 (3%)	49	25	49, 93, 161, 203	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	382	THR	9.6
5	F	376	ILE	9.3
2	C	770	GLU	9.2
5	F	377	ASP	9.1
5	F	381	HIS	9.0
5	F	404	ALA	7.9
2	C	769	PRO	7.8
5	F	383	LEU	7.6
5	F	387	GLY	7.4
5	F	403	LYS	7.3
5	F	375	LEU	6.8
5	F	386	VAL	6.6
5	F	370	LYS	6.4
5	F	388	ALA	6.1
5	F	392	VAL	5.8
5	F	356	LYS	5.6

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Mol	Chain	Res	Type	RSRZ
5	F	389	PHE	5.6
5	F	359	SER	5.5
5	F	401	GLU	5.4
2	C	64	LEU	5.3
5	F	367	MET	5.0
5	F	357	ALA	4.8
5	F	149	GLU	4.8
5	F	353	GLU	4.7
5	F	397	ILE	4.7
5	F	390	PHE	4.6
5	F	414	ARG	4.6
2	C	766	GLU	4.4
5	F	360	LYS	4.4
5	F	393	THR	4.3
2	C	773	LEU	4.2
5	F	399	GLN	4.0
5	F	413	SER	4.0
5	F	391	GLY	4.0
5	F	379	ARG	3.7
5	F	400	ILE	3.7
5	F	369	LEU	3.6
3	D	241	ILE	3.6
2	C	362	GLY	3.6
5	F	150	THR	3.6
3	D	1238	MET	3.5
3	D	1313	VAL	3.4
2	C	221	LEU	3.3
3	D	1287	GLU	3.2
3	D	1297	GLU	3.2
2	C	772	ARG	3.1
3	D	1499	ARG	3.1
2	C	104	ASP	3.1
2	C	217	LEU	3.1
5	F	323	ASP	3.1
5	F	385	GLU	3.0
5	F	361	LEU	3.0
2	C	420	ARG	3.0
2	C	207	LEU	3.0
5	F	374	GLY	2.9
2	C	311	PHE	2.9
2	C	776	SER	2.9
2	C	189	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	811	PRO	2.8
2	C	219	GLN	2.8
3	D	1319	VAL	2.8
2	C	153	ALA	2.7
2	C	242	LEU	2.7
2	C	181	VAL	2.7
3	D	310	LEU	2.7
3	D	1502	ALA	2.6
3	D	350	HIS	2.6
5	F	416	ARG	2.5
2	C	245	GLY	2.5
3	D	322	VAL	2.5
5	F	362	SER	2.5
5	F	365	GLU	2.5
5	F	349	LEU	2.5
2	C	511	GLU	2.5
2	C	176	VAL	2.5
6	G	20	DG	2.5
2	C	216	GLU	2.4
2	C	103	LYS	2.4
5	F	422	LEU	2.4
3	D	983	LEU	2.4
3	D	1300	SER	2.4
3	D	1278	ASP	2.4
2	C	298	PHE	2.3
3	D	1128	VAL	2.3
3	D	1318	TYR	2.3
3	D	1497	GLU	2.3
2	C	243	ARG	2.3
2	C	617	ASP	2.3
3	D	360	ARG	2.3
3	D	170	PRO	2.2
2	C	361	MET	2.2
2	C	251	ASP	2.2
7	H	11	DC	2.2
3	D	1495	ILE	2.2
7	H	25	DG	2.2
2	C	372	LEU	2.2
5	F	373	LYS	2.2
5	F	415	THR	2.1
5	F	396	ARG	2.1
2	C	109	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
5	F	364	ARG	2.1
5	F	148	LYS	2.1
5	F	371	LEU	2.1
5	F	407	LYS	2.1
3	D	1288	GLU	2.1
2	C	365	ASP	2.1
3	D	1306	PRO	2.1
3	D	324	ALA	2.1
3	D	1493	LYS	2.0
2	C	419	THR	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
8	MG	G	101	1/1	0.51	0.34	113,113,113,113	0
9	ZN	D	2001	1/1	0.97	0.18	96,96,96,96	0
8	MG	D	2003	1/1	0.98	0.36	50,50,50,50	0
8	MG	B	401	1/1	0.99	0.39	69,69,69,69	0
9	ZN	D	2002	1/1	1.00	0.08	124,124,124,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.