



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 05:46 AM BST

PDB ID : 6CCV  
Title : Crystal structure of a Mycobacterium smegmatis RNA polymerase transcription initiation complex with inhibitor Rifampicin  
Authors : Lilic, M.; Darst, S.A.; Campbell, E.A.  
Deposited on : 2018-02-07  
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](mailto: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.

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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 : 2.14.4.dev1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

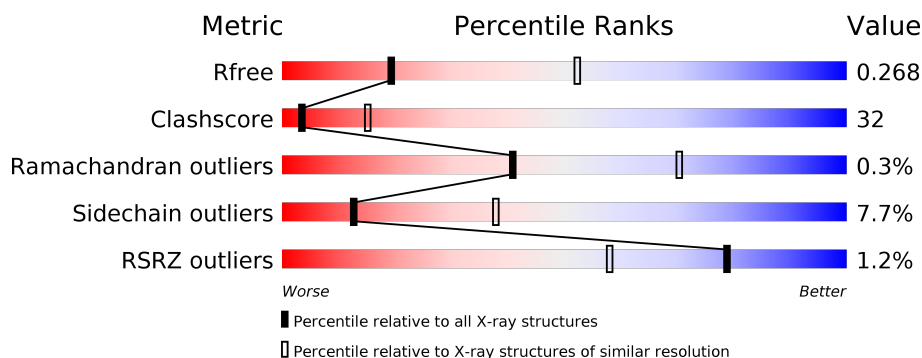
# 1 Overall quality at a glance

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.



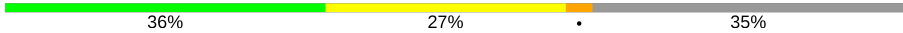



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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  $\geq 3$ , 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	350	
1	B	350	
1	T	350	
2	C	1169	
3	D	1317	
4	E	107	

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Mol	Chain	Length	Quality of chain
5	F	466	
6	G	17	
7	J	114	
8	O	31	
9	P	26	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SO4	D	2004	-	-	X	-
11	EDO	F	506	-	-	-	X
14	GLU	D	2012	-	-	X	-

## 2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 26582 atoms, of which 48 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	218	Total	C	N	O	S	0	0	0
			1605	1015	276	311	3			
1	B	233	Total	C	N	O	S	0	0	0
			1667	1054	289	322	2			
1	T	53	Total	C	N	O	S	0	0	0
			342	208	65	68	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1099	Total	C	N	O	S	0	0	0
			8262	5174	1450	1603	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1246	Total	C	N	O	S	0	0	0
			9555	5995	1720	1800	40			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	76	Total	C	N	O	0	0	0
			592	378	100	114			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	305	Total	C	N	O	S	0	0	0
			2414	1512	436	459	7			

- Molecule 6 is a protein called Unknown Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	17	Total	C	N	O	0	0	0
			85	51	17	17			

- Molecule 7 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	83	Total	C	N	O	S	0	0	0
			671	422	119	128	2			

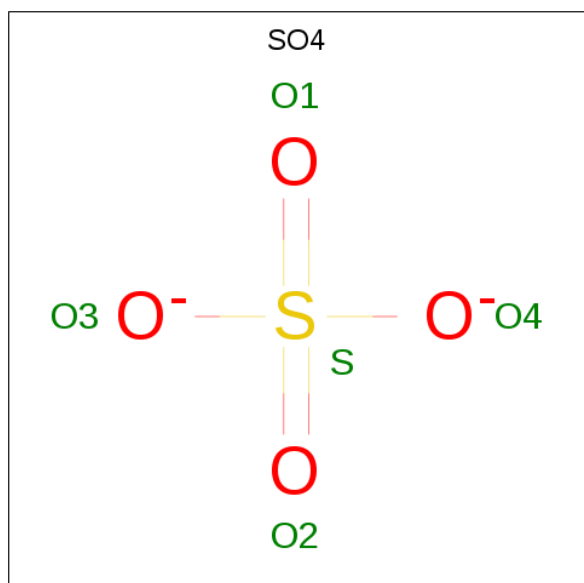
- Molecule 8 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	O	31	Total	C	N	O	P	0	0	0
			634	305	114	185	30			

- Molecule 9 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



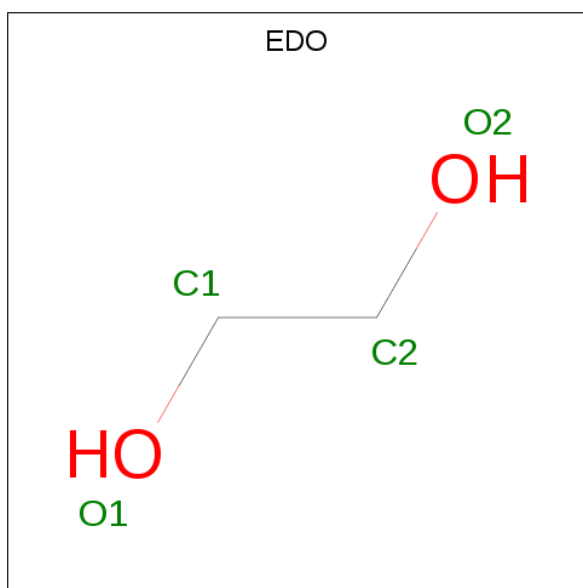
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		

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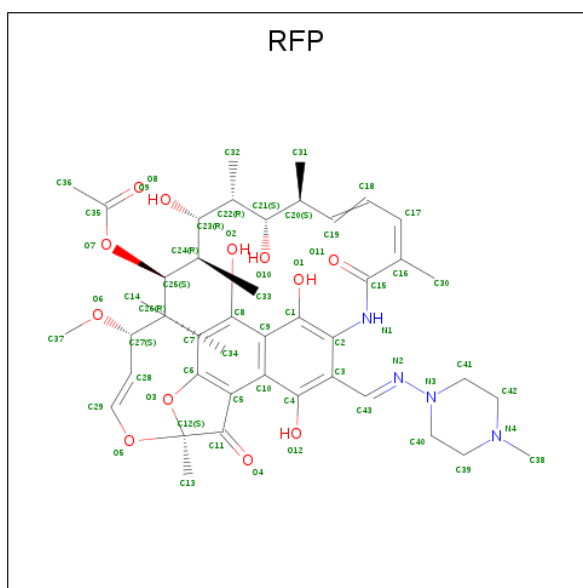
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	C	1	Total C H O 10 2 6 2	0	0
11	C	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	D	1	Total C H O 10 2 6 2	0	0
11	F	1	Total C H O 10 2 6 2	0	0
11	F	1	Total C H O 10 2 6 2	0	0

- Molecule 12 is RIFAMPICIN (three-letter code: RFP) (formula:  $C_{43}H_{58}N_4O_{12}$ ).

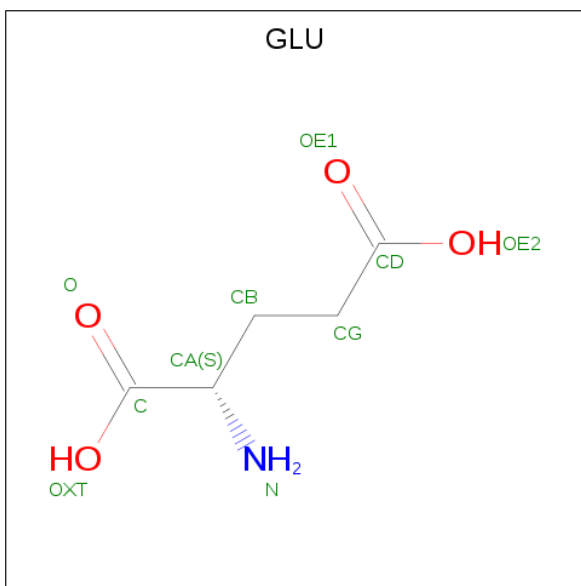


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	C	1	Total C N O 59 43 4 12	0	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 14 is GLUTAMIC ACID (three-letter code: GLU) (formula:  $C_5H_9NO_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	D	1	Total	C	N	O	0	0
			9	5	1	3		

- Molecule 15 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	C	5	Total	O	0	0
			5	5		
15	D	8	Total	O	0	0
			8	8		
15	F	1	Total	O	0	0
			1	1		





[illegible]

- Molecule 1: DNA-directed RNA polymerase subunit alpha



NET	LEU	ILE	SER	GLN	ARG	PRO	THR	LEU	SER	SER	GLU	THR	VAL	ALA	GLU	ASN	ARG	SER	ARG	PHE	VAL	ILE	GLU	PRO	LEU	GLY	GLY	TYR	THR	LEU	GLY	ASN	SER	SER	LEU	ARG	ARG	ARG	LEU	LEU	THR	THR	ILE	ARG	ILE	ILE	ASP	GLY	VAL	LEU
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HIS	GLU	PHE	THR	THR	VAL	PRO	GLY	VAL	LYS	ASP	GLU	THR	THR	ASP	ASP	GLY	LEU	VAL	VAL	VAL	SER	SER	ASP	ASP	ASP	GLU	PRO	GLU	VAL	THR	THR	MET	THR	LEU	ARG	LYS	GLN	GLY	GLY	PRO	GLY	VAL	THR	THR	ALA	ALA	ASP	ASP	ILE	VAL	PRO	PRO	PRO	ALA	ALA	GLY	VAL	THR	THR	THR	HIS	ASN
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PRO	ASP	MET	HIS	ILE	ALA	THR	LEU	ASN	ASP	LYS	GLY	LYS	LEU	GLU	VAL	GLU	GLU	VAL	VAL	VAL	VAL	VAL	PRO	PRO	ALA	VAL	GLN	ASN	LYS	LYS	ALA	ALA	SER	SER	GLY	GLY	ALA	GLU	GLU	ILE	ILE	GLY	ARG	ARG	ILE	ILE	PRO	VAL	VAL	ASP	SER	ASP	ILE	TYR	TYR	SER	PRO	VAL	VAL	LYS	VAL	VAL	GLU	ALA
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THR	ARG	VAL	GLU	GLN	ARG	THR	ASP	PHE	ASP	LYS	LEU	ILE	ILE	ASP	VAL	GLU	THR	LYS	ASN	SER	ILE	SER	PRO	ARG	ASP	ALA	LEU	ALA	SER	GLY	GLY	THR	LEU	VAL	LEU	GLU	LEU	PHE	GLY	GLY	ALA	ALA	ASN	LEU	GLU	GLY	GLU	THR	PRO	SER	HIS	ILE	ILE	GLU	ILE	GLY	PRO	SER	PRO	ALA	GLU
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[illegible]

ALA  
GLY  
TYR  
ASP  
ALA  
ALA  
THR  
GLY  
THR  
TRP  
THR  
SER  
ASP  
ALA  
GLY  
TYR  
ASP  
LEU  
ASP  
ASP  
ASN  
GLN  
ASP  
TYR  
ALA  
GLU  
THR  
GLU  
GLN  
LEU

- Molecule 2: DNA-directed RNA polymerase subunit beta



MET	LEU	GLU	GLY	CYS	ILE	LEU	ALA	VAL	SER	SER	GLN	SER	LYS	SER	ASN	ASN	N21	N22	V23		A26		R29	V30	S31	F32	A33	K34	K35	R36	F37	P38		V41	L44	L45		S51	F52	E53			G57		R60		A65	I66	D67		E70		G76		V80
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S85	P86	R87	E88	G92	S93	M94	L95	D100	P101	R102	V106	K114	T119	Y120	P123	L124	F125	V126	T127	A128	E129	M132	M133	T134	T135	G136	K139	A140	Q141	T142	V143	F144	F148	P149	M150	M151	T152	E153	K154	G155	I158	L159	M160	G161	V166	V167	S169
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Q169	L170	L171	R172	S173	P174	G175	V176	F177	F178	D179	E180	T181	S185	T186	F187	K188	T189	V193	K194	V195	T196	R199	N202	L203	E204	F205	ASP	VAL	ASP	ASP	LYS	ARG	ASP	THR	VAL	GLY	T215	R216	L217	R221	R222	Q223	Q224	V225	T226	V227	L228	L229	R230	A231	L232	G233	G234	T235	T236
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Category	Value
T239	1239
S246	246
K249	249
M250	250
L253	253
T261	261
D262	262
L265	265
L268	268
Y269	269
L272	272
R273	273
P274	274
G275	275
P278	278
L279	279
K280	280
Q284	284
L287	287
F291	291
E294	294
K295	295
L299	299
A300	300
R301	301
V302	302
K306	306
V307	307
K310	310
L311	311
GLY	311
LEU	311
ASN	311
ALA	311
GLY	311
LVS	311
PRO	311
ILE	311
THR	311
SER	311
SER	311
T323	323
L324	324
P235	235

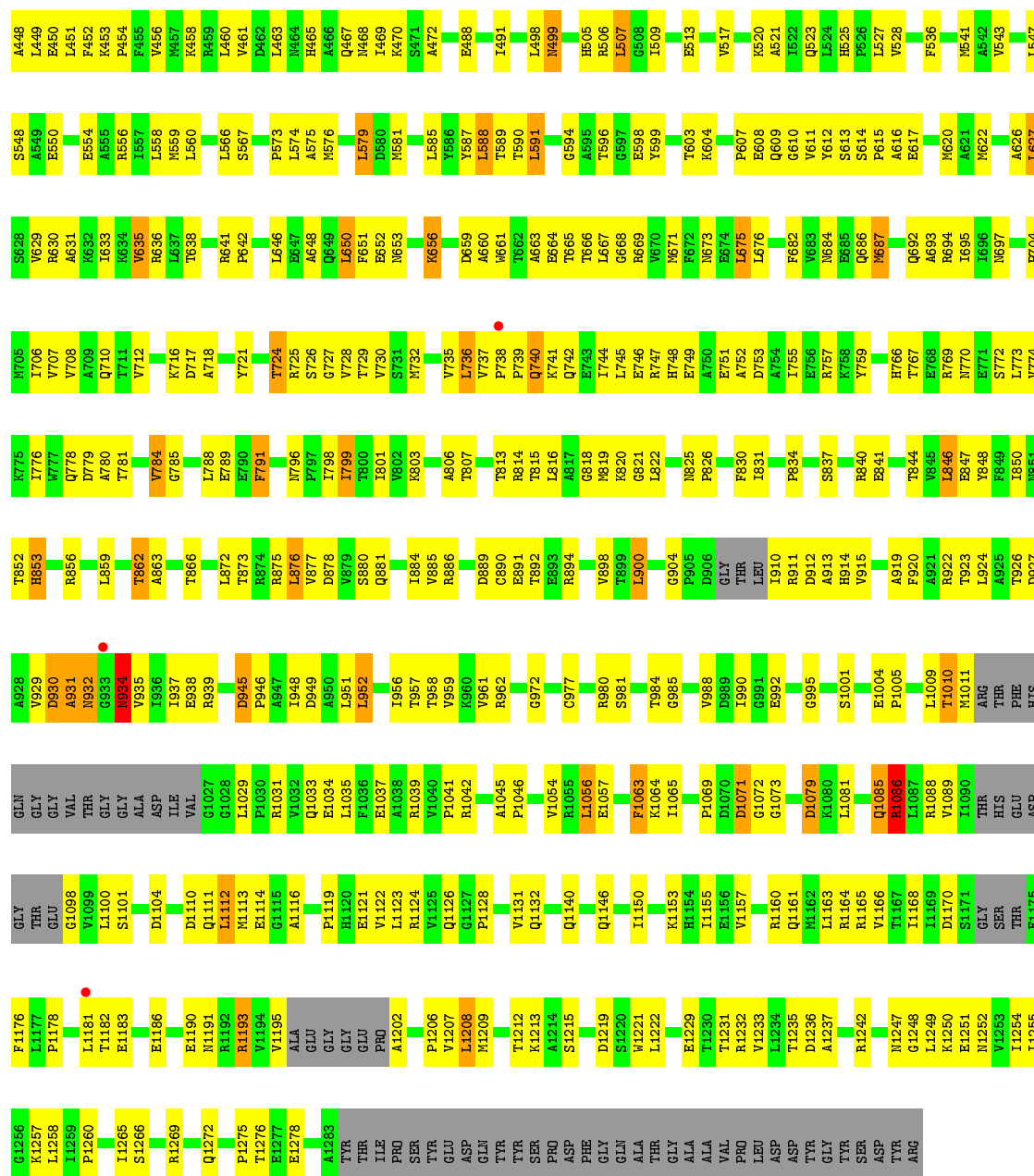
D328	T332	T333	E334	Y335	T336	V337	R338	Q343	T344	S345	M346	T347	V348	P349	P349	G350	G351	V352	E353	V354	P355	V358	I361	N366	R370	T371	V372	G373	E374	T375	I376	Q379	I380	M387	E388	R389	V390	V391	R392	E393	R394	M395	Q398	E401	A402	I403	T404	P405	O406
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T407	I411	R412	I418	F421	F422	S425	Q426	L427	S428	Q429	D432	Q433	M434	M435	P436	L437	L440	T441	H442	K443	R444	R445	L446	S447	A448	L449	G450	L454	S455	R456	A459	V466	H467	P468	G472	R473	M474	C475	P476	P477	I477	E478	T479	P480	E481	G482	L485
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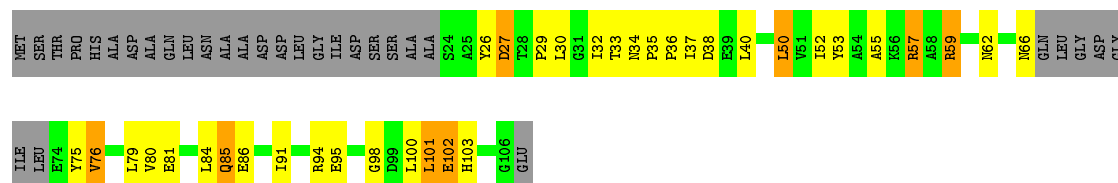
Chain D:  50% 40% 5%





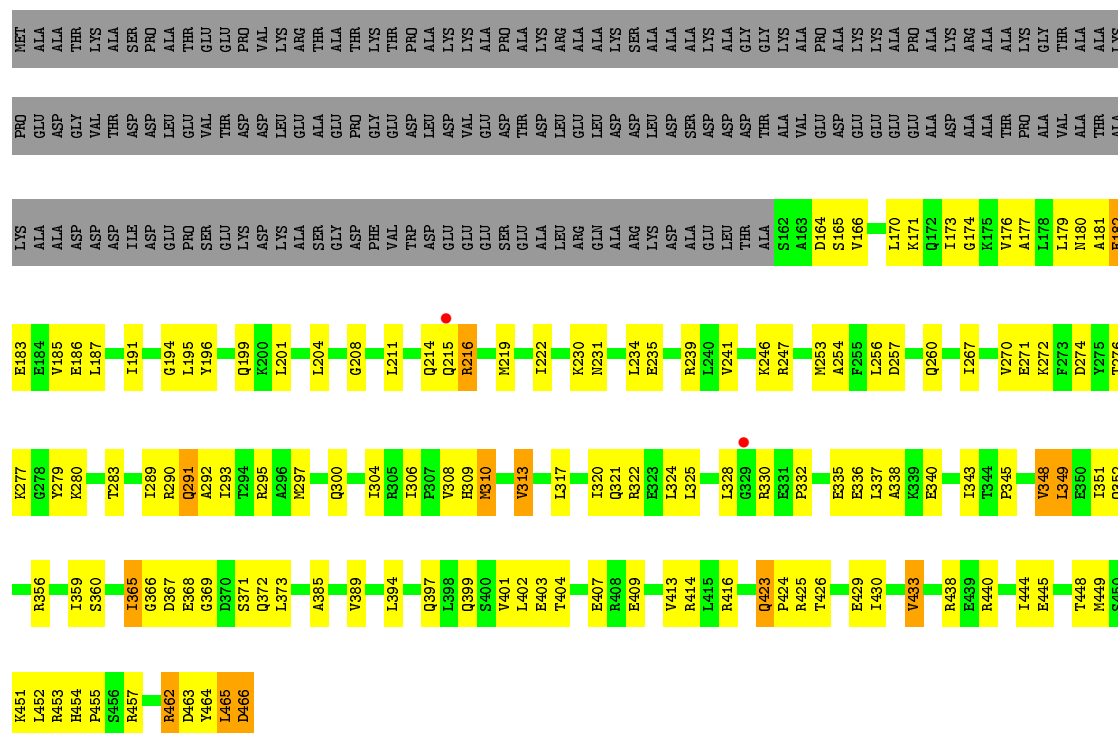
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 37% 26% 7% 29%



• Molecule 5: RNA polymerase sigma factor SigA

Chain F: 36% 27% 35%



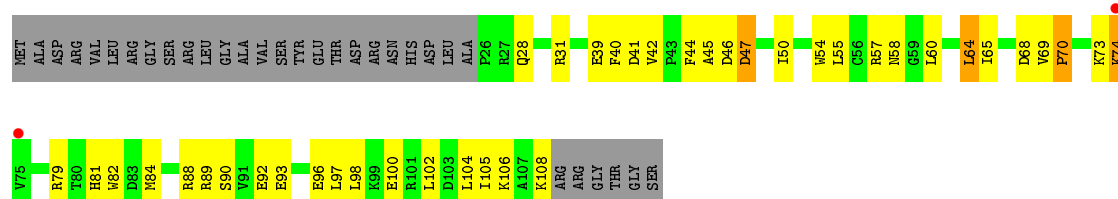
● Molecule 6: Unknown Peptide

Chain G:  100%

There are no outlier residues recorded for this chain.

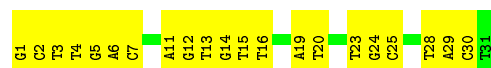
● Molecule 7: RNA polymerase-binding protein RbpA

Chain J:  37% 32% 27%



● Molecule 8: DNA (31-MER)

Chain O:  32% 68%



● Molecule 9: DNA (26-MER)

Chain P:  62% 38%

A1	G2	C3	A4	C5	A11	A12	T17	G20	T21	G22	A23	A24	G25	C26
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.35Å 162.32Å 139.40Å 90.00° 107.37° 90.00°	Depositor
Resolution (Å)	57.12 – 3.05 57.12 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.0 (57.12-3.05) 88.8 (57.12-2.88)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.22 (at 2.86Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.223 , 0.269 0.223 , 0.268	Depositor DCC
$R_{free}$ test set	1877 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.8	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 61.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	26582	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, RFP, SO4, EDO

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	0.23	0/1629	0.45	0/2220
1	B	0.23	0/1693	0.43	0/2316
1	T	0.22	0/343	0.37	0/468
2	C	0.24	0/8408	0.43	0/11428
3	D	0.24	0/9706	0.43	1/13140 (0.0%)
4	E	0.24	0/604	0.43	0/822
5	F	0.22	0/2445	0.39	0/3300
7	J	0.23	0/685	0.42	0/927
8	O	0.51	0/710	0.94	0/1095
9	P	0.57	0/589	0.93	0/906
All	All	0.26	0/26812	0.47	1/36622 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	5
3	D	0	3
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	579	LEU	CA-CB-CG	5.98	129.06	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	C	1133	GLY	Peptide
2	C	324	LEU	Peptide
2	C	540	ASP	Peptide
2	C	985	PRO	Peptide
2	C	986	ASN	Peptide
3	D	1085	GLN	Peptide
3	D	1193	ARG	Peptide
3	D	934	ASN	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	1605	0	1623	141	0
1	B	1667	0	1636	166	0
1	T	342	0	275	15	0
2	C	8262	0	8009	627	1
3	D	9555	0	9509	600	1
4	E	592	0	583	40	0
5	F	2414	0	2434	151	0
6	G	85	0	19	0	0
7	J	671	0	660	48	0
8	O	634	0	350	40	0
9	P	526	0	296	15	0
10	C	20	0	0	3	0
10	D	25	0	0	3	0
10	F	20	0	0	1	0
11	C	8	12	12	0	0
11	D	16	24	24	3	0
11	F	8	12	12	3	0
12	C	59	0	58	9	0
13	D	2	0	0	0	0
14	D	9	0	5	10	0
15	C	5	0	0	0	0
15	D	8	0	0	1	0
15	F	1	0	0	0	0
All	All	26534	48	25505	1669	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 32.

All (1669) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:603:THR:HG22	3:D:604:LYS:HG3	1.19	1.15
1:A:197:GLU:OE1	2:C:987:ARG:NH1	1.87	1.07
2:C:203:LEU:HG	2:C:217:ILE:HG22	1.35	1.07
2:C:771:VAL:HG22	2:C:772:LEU:HD12	1.35	1.07
2:C:53:GLU:OE2	2:C:60:ARG:NH1	1.89	1.06
3:D:1266:SER:HB3	14:D:2012:GLU:HG3	1.37	1.04
3:D:1009:LEU:HD12	3:D:1146:GLN:HG3	1.36	1.04
7:J:106:LYS:HA	7:J:106:LYS:HE2	1.38	1.03
3:D:929:VAL:HG12	3:D:935:VAL:HG22	1.34	1.03
2:C:710:LEU:HD22	2:C:1021:ILE:HD11	1.38	1.02
5:F:324:LEU:HD22	5:F:332:PRO:HB3	1.43	1.01
1:A:177:LYS:HE2	1:A:193:ILE:HD11	1.41	1.01
3:D:951:LEU:HB3	3:D:956:ILE:HD11	1.40	1.00
3:D:922:ARG:HB3	3:D:961:VAL:HG21	1.40	1.00
3:D:656:LYS:HE3	3:D:656:LYS:H	1.26	0.99
3:D:288:LYS:HD2	3:D:291:ARG:HH21	1.26	0.99
2:C:204:GLU:OE1	2:C:216:ARG:NH1	1.96	0.98
3:D:755:ILE:HD12	3:D:776:ILE:HD11	1.45	0.97
2:C:348:VAL:HB	2:C:349:PRO:HD2	1.46	0.96
2:C:602:MET:HE1	2:C:883:LYS:HB3	1.48	0.96
3:D:59:GLU:OE2	3:D:66:LYS:NZ	2.00	0.95
7:J:68:ASP:HA	7:J:69:VAL:HB	1.47	0.95
2:C:758:GLU:HG2	2:C:798:THR:HG22	1.49	0.95
3:D:432:VAL:HG22	3:D:434:PRO:HD3	1.49	0.95
2:C:176:VAL:HG12	2:C:195:VAL:HG22	1.45	0.94
2:C:540:ASP:HB2	2:C:546:THR:HG22	1.50	0.94
2:C:649:ILE:HD11	2:C:679:PRO:HB3	1.48	0.93
2:C:624:ARG:NH1	2:C:628:ASP:OD2	2.01	0.93
3:D:1265:ILE:HG23	14:D:2012:GLU:HG2	1.48	0.93
1:T:252:ASP:OD2	1:T:261:TYR:OH	1.86	0.93
2:C:635:ALA:HB2	2:C:693:ILE:HD11	1.51	0.92
5:F:308:VAL:HG21	8:O:23:DT:H71	1.51	0.92
3:D:581:MET:HE2	3:D:716:LYS:HA	1.52	0.91
5:F:253:MET:HE2	5:F:300:GLN:HB2	1.49	0.91
1:A:1:MET:N	1:B:142:ARG:O	2.03	0.91
2:C:984:LEU:HD13	2:C:991:VAL:HG23	1.52	0.91
3:D:400:LYS:HE2	3:D:405:LEU:HD23	1.51	0.91
2:C:1045:GLN:HG2	2:C:1087:THR:HG22	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:438:ARG:NH1	9:P:20:DG:N7	2.19	0.90
3:D:47:PHE:O	3:D:88:ARG:NH2	2.04	0.90
2:C:444:ARG:HH21	2:C:491:LEU:HD23	1.35	0.89
1:A:31:GLY:HA2	1:A:192:LEU:HD23	1.54	0.89
2:C:531:VAL:HG13	2:C:552:VAL:HG13	1.55	0.88
1:B:24:GLU:OE2	1:B:191:LYS:HD3	1.73	0.88
2:C:132:ASN:HB3	2:C:135:THR:HG22	1.56	0.87
2:C:799:PRO:HA	2:C:823:VAL:HG12	1.56	0.87
3:D:1232:ARG:NH1	3:D:1236:ASP:OD2	2.07	0.86
2:C:1048:LEU:HD23	2:C:1048:LEU:H	1.40	0.86
2:C:215:VAL:HG22	2:C:225:VAL:HA	1.56	0.86
3:D:627:LEU:HD13	3:D:667:LEU:HD12	1.57	0.86
2:C:394:ARG:HG3	2:C:398:GLN:HG3	1.54	0.86
1:A:152:ASN:HB2	1:A:157:ALA:HB3	1.56	0.86
3:D:710:GLN:OE1	4:E:27:ASP:HB2	1.74	0.86
2:C:88:GLU:HG2	2:C:92:GLY:HA2	1.57	0.86
2:C:92:GLY:O	2:C:133:ASN:ND2	2.08	0.86
3:D:579:LEU:HD23	3:D:807:THR:HB	1.57	0.86
5:F:324:LEU:HD23	5:F:328:LEU:HD13	1.58	0.86
2:C:584:MET:HA	2:C:619:THR:HG21	1.56	0.85
4:E:86:GLU:OE2	4:E:94:ARG:NH1	2.09	0.85
1:B:9:LEU:HD21	1:B:208:LEU:HD21	1.56	0.85
2:C:41:VAL:O	2:C:624:ARG:NH2	2.09	0.84
5:F:399:GLN:NE2	5:F:403:GLU:OE2	2.10	0.84
1:A:40:ARG:NH1	1:B:33:THR:HG22	1.93	0.84
2:C:1100:GLY:HA3	3:D:458:LYS:HE3	1.58	0.83
3:D:417:LEU:HG	3:D:1254:ILE:HG23	1.60	0.83
3:D:886:ARG:HH12	14:D:2012:GLU:HA	1.43	0.83
3:D:603:THR:CG2	3:D:604:LYS:HG3	2.07	0.83
2:C:711:LEU:HD23	2:C:904:VAL:HA	1.60	0.83
3:D:1265:ILE:CG2	14:D:2012:GLU:HG2	2.09	0.83
1:A:40:ARG:HD3	1:B:33:THR:HG22	1.61	0.83
1:B:95:MET:HG2	1:B:113:PRO:HD2	1.60	0.83
3:D:642:PRO:HD3	3:D:656:LYS:HD2	1.59	0.83
5:F:320:ILE:HG23	5:F:340:GLU:HG2	1.60	0.83
2:C:763:ASP:HB3	2:C:821:ARG:HH22	1.43	0.82
7:J:31:ARG:NH2	7:J:39:GLU:OE1	2.13	0.82
3:D:1248:GLY:O	3:D:1252:ASN:ND2	2.13	0.82
3:D:590:THR:HG21	3:D:630:ARG:HH21	1.45	0.82
2:C:773:ALA:O	2:C:782:ARG:NH2	2.13	0.81
3:D:922:ARG:HB3	3:D:961:VAL:CG2	2.10	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:910:THR:HG23	3:D:730:VAL:HG23	1.62	0.80
2:C:51:SER:OG	2:C:373:GLY:N	2.13	0.80
2:C:404:THR:HG22	2:C:407:THR:HG23	1.63	0.80
3:D:706:ILE:HD12	4:E:36:PRO:HB3	1.63	0.80
5:F:253:MET:HE3	5:F:297:MET:HA	1.63	0.80
1:A:40:ARG:HH11	1:B:33:THR:HG22	1.46	0.80
1:B:100:GLN:HA	1:B:133:LYS:HA	1.63	0.80
4:E:84:LEU:H	4:E:84:LEU:HD12	1.47	0.79
1:T:251:ILE:HA	1:T:272:VAL:HG22	1.61	0.79
3:D:1088:ARG:HG2	3:D:1089:VAL:H	1.44	0.79
1:A:113:PRO:HD2	1:A:116:VAL:HG21	1.65	0.79
1:B:3:ILE:HA	1:B:232:ILE:CB	2.13	0.78
3:D:892:THR:OG1	3:D:894:ARG:NH1	2.13	0.78
5:F:368:GLU:HG2	5:F:369:GLY:H	1.47	0.78
1:B:47:PRO:HA	1:B:144:ARG:HG3	1.65	0.78
3:D:1079:ASP:N	3:D:1079:ASP:OD1	2.16	0.78
3:D:12:ILE:HD11	3:D:1221:TRP:CD2	2.19	0.78
2:C:574:PRO:O	2:C:575:ARG:HG2	1.83	0.78
1:A:56:ILE:HG12	1:A:136:VAL:HB	1.66	0.78
2:C:578:VAL:HG13	2:C:582:THR:HB	1.66	0.78
3:D:1164:ARG:NH1	10:D:2004:SO4:O1	2.17	0.77
1:B:84:VAL:HB	1:B:199:LYS:HD3	1.65	0.77
3:D:603:THR:HG22	3:D:604:LYS:CG	2.10	0.77
12:C:1205:RFP:H392	10:C:1206:SO4:O4	1.85	0.77
3:D:735:VAL:HG12	3:D:840:ARG:HD2	1.66	0.77
4:E:84:LEU:HB2	4:E:85:GLN:HE21	1.48	0.77
8:O:14:DG:H2''	8:O:15:DT:OP2	1.84	0.77
8:O:19:DA:H2''	8:O:20:DT:O5'	1.85	0.77
3:D:327:MET:HE2	5:F:304:ILE:HD11	1.65	0.77
2:C:590:HIS:HB3	2:C:919:ILE:CD1	2.15	0.76
3:D:1275:PRO:HG3	4:E:76:VAL:HG11	1.68	0.76
1:B:74:THR:HG21	3:D:611:VAL:HG11	1.67	0.76
1:A:98:ARG:HG2	1:A:135:GLU:HG2	1.68	0.76
3:D:1009:LEU:CD1	3:D:1146:GLN:HG3	2.15	0.76
2:C:150:MET:HE2	2:C:150:MET:HA	1.68	0.76
3:D:607:PRO:O	3:D:609:GLN:HG2	1.85	0.76
3:D:588:LEU:HD22	3:D:668:GLY:HA3	1.67	0.75
3:D:815:THR:HG22	3:D:820:LYS:HA	1.68	0.75
2:C:448:ALA:HB1	2:C:454:LEU:HD11	1.67	0.75
2:C:935:TRP:HB2	2:C:982:SER:HB3	1.68	0.75
2:C:265:LEU:HD21	2:C:284:GLN:HA	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1275:PRO:HB3	4:E:79:LEU:HD11	1.69	0.75
3:D:327:MET:HG3	3:D:337:THR:HB	1.69	0.75
3:D:21:ARG:NE	3:D:96:GLU:OE2	2.18	0.75
2:C:299:LEU:HB3	2:C:323:THR:HB	1.68	0.75
1:A:38:LEU:HD13	1:A:208:LEU:HD11	1.68	0.75
3:D:962:ARG:NH1	3:D:977:CYS:SG	2.59	0.75
3:D:1086:ARG:HD2	3:D:1086:ARG:H	1.51	0.74
3:D:1276:THR:HG22	4:E:102:GLU:HG3	1.69	0.74
5:F:280:LYS:HG2	8:O:30:DC:OP2	1.87	0.74
1:A:70:LYS:HB3	1:A:127:THR:HG23	1.67	0.74
3:D:721:TYR:O	3:D:725:ARG:HG2	1.86	0.74
8:O:15:DT:OP1	1:T:258:VAL:HG21	1.87	0.74
8:O:12:DG:H2"	8:O:13:DT:H5'	1.70	0.74
1:A:14:VAL:HG13	1:A:18:ARG:HG3	1.68	0.74
2:C:568:ASP:N	2:C:568:ASP:OD1	2.20	0.74
3:D:796:ASN:HD21	3:D:798:ILE:HB	1.51	0.74
2:C:1127:GLU:OE1	3:D:11:ARG:NH2	2.20	0.74
2:C:1129:LEU:HA	2:C:1134:ALA:O	1.87	0.74
3:D:1041:PRO:HB3	3:D:1116:ALA:HB3	1.69	0.74
8:O:6:DA:H2"	8:O:7:DC:H5'	1.67	0.74
2:C:754:LYS:HE2	2:C:754:LYS:H	1.53	0.73
3:D:365:ILE:HD12	3:D:365:ILE:H	1.51	0.73
3:D:781:THR:HG22	3:D:814:ARG:HD2	1.68	0.73
3:D:937:ILE:HD12	3:D:951:LEU:HG	1.69	0.73
3:D:922:ARG:CB	3:D:961:VAL:HG21	2.18	0.73
1:A:66:VAL:O	1:A:69:VAL:HG22	1.88	0.73
2:C:732:LEU:HD22	2:C:737:VAL:HG11	1.69	0.73
3:D:641:ARG:HA	3:D:656:LYS:NZ	2.03	0.73
1:B:24:GLU:OE2	1:B:181:THR:HG21	1.89	0.73
2:C:324:LEU:O	2:C:324:LEU:HD22	1.88	0.73
3:D:924:LEU:HD21	3:D:959:VAL:HG13	1.70	0.73
4:E:30:LEU:O	4:E:33:THR:HG22	1.88	0.72
3:D:1168:ILE:HD13	3:D:1176:PHE:HB3	1.69	0.72
2:C:508:ARG:HD3	2:C:515:VAL:HG11	1.70	0.72
2:C:729:SER:HA	2:C:895:MET:HE1	1.72	0.72
2:C:510:VAL:N	2:C:568:ASP:O	2.18	0.72
3:D:1071:ASP:HB2	3:D:1073:GLY:N	2.05	0.72
2:C:429:GLN:HG2	12:C:1205:RFP:H343	1.71	0.72
2:C:224:PRO:O	2:C:227:VAL:HG22	1.90	0.72
5:F:462:ARG:HH12	5:F:465:LEU:HD12	1.55	0.71
3:D:622:MET:HE3	3:D:667:LEU:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:11:DA:H2''	9:P:12:DA:O5'	1.90	0.71
2:C:482:GLY:O	2:C:485:ILE:HG13	1.90	0.71
3:D:453:LYS:HB3	3:D:454:PRO:HD3	1.72	0.71
2:C:589:GLU:OE1	2:C:589:GLU:N	2.22	0.71
2:C:1108:ILE:H	2:C:1108:ILE:HD12	1.55	0.71
2:C:891:PRO:HB2	2:C:893:GLU:HG2	1.72	0.71
3:D:111:PRO:O	3:D:113:ARG:NH1	2.24	0.70
3:D:190:LYS:NZ	3:D:192:ASP:HB3	2.06	0.70
3:D:277:LEU:HD11	3:D:295:ARG:HG2	1.73	0.70
2:C:176:VAL:HG22	2:C:307:VAL:HG12	1.71	0.70
2:C:764:ILE:HB	2:C:767:VAL:HG21	1.73	0.70
8:O:14:DG:H3'	1:T:258:VAL:HG11	1.73	0.70
3:D:951:LEU:HB3	3:D:956:ILE:CD1	2.20	0.70
2:C:96:LEU:HA	2:C:129:GLU:O	1.91	0.70
2:C:797:VAL:HG12	2:C:823:VAL:HB	1.72	0.70
3:D:596:THR:HG22	3:D:626:ALA:O	1.92	0.69
3:D:642:PRO:CD	3:D:656:LYS:HD2	2.21	0.69
2:C:650:THR:HG22	2:C:660:SER:OG	1.91	0.69
3:D:1081:LEU:HB3	3:D:1113:MET:HE1	1.73	0.69
3:D:735:VAL:HG22	3:D:798:ILE:HD11	1.74	0.69
2:C:894:ASP:HA	2:C:1004:GLY:HA3	1.74	0.69
2:C:1128:VAL:HG13	2:C:1136:ILE:HB	1.74	0.69
2:C:637:LYS:HD2	2:C:659:GLN:NE2	2.07	0.69
3:D:1009:LEU:HD12	3:D:1146:GLN:CG	2.18	0.69
1:A:36:ASN:HB2	1:A:176:TYR:OH	1.93	0.69
2:C:302:VAL:O	2:C:306:LYS:HG2	1.91	0.69
2:C:41:VAL:HG22	2:C:494:TYR:HE1	1.57	0.69
2:C:804:GLU:HG3	3:D:66:LYS:HE3	1.74	0.69
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.72	0.69
5:F:253:MET:CE	5:F:300:GLN:HB2	2.21	0.69
3:D:641:ARG:HA	3:D:656:LYS:HZ3	1.57	0.69
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.74	0.69
4:E:62:ASN:O	4:E:66:ASN:ND2	2.26	0.69
2:C:379:GLN:HG2	2:C:421:PHE:HB2	1.75	0.69
3:D:735:VAL:HG22	3:D:798:ILE:CD1	2.23	0.69
3:D:911:ARG:NH1	3:D:949:ASP:OD1	2.24	0.69
5:F:201:LEU:HD11	5:F:219:MET:HB3	1.75	0.68
2:C:215:VAL:O	2:C:223:GLN:HB2	1.93	0.68
2:C:984:LEU:HB3	2:C:991:VAL:HG22	1.74	0.68
3:D:73:ILE:O	3:D:82:VAL:HG12	1.93	0.68
3:D:772:SER:O	3:D:776:ILE:HG13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:895:MET:HG3	2:C:896:PRO:HD2	1.74	0.68
2:C:361:ILE:H	2:C:361:ILE:HD12	1.59	0.68
3:D:929:VAL:HG12	3:D:935:VAL:CG2	2.18	0.68
2:C:742:HIS:CD2	2:C:868:ARG:HG3	2.28	0.68
2:C:94:MET:CE	2:C:395:MET:HB3	2.23	0.68
3:D:1247:ASN:O	3:D:1260:PRO:HG3	1.94	0.68
2:C:602:MET:HE2	2:C:1024:LEU:HD21	1.74	0.68
5:F:454:HIS:ND1	5:F:455:PRO:HD2	2.08	0.68
1:B:74:THR:CG2	3:D:611:VAL:HG11	2.23	0.68
2:C:623:LEU:HA	2:C:703:GLU:HA	1.75	0.68
5:F:330:ARG:NH2	5:F:336:GLU:OE2	2.26	0.68
2:C:494:TYR:HB3	2:C:506:PRO:HG3	1.75	0.68
2:C:1098:VAL:HG11	3:D:469:ILE:HD12	1.75	0.67
2:C:1003:ASP:OD1	2:C:1006:SER:N	2.23	0.67
2:C:921:GLN:HB2	2:C:1019:MET:HE1	1.76	0.67
2:C:333:ILE:O	2:C:337:VAL:HG23	1.94	0.67
2:C:768:SER:O	2:C:771:VAL:HG13	1.93	0.67
3:D:1122:VAL:HG23	3:D:1126:GLN:HE21	1.59	0.67
1:B:79:ASN:OD1	3:D:636:ARG:NH2	2.27	0.67
1:T:264:LEU:HB3	1:T:269:VAL:CG2	2.24	0.67
1:B:107:ALA:O	1:B:110:ILE:HG22	1.93	0.67
2:C:771:VAL:HG23	2:C:792:ILE:HD13	1.76	0.67
1:A:177:LYS:HE2	1:A:193:ILE:CD1	2.22	0.67
3:D:70:PHE:HB2	3:D:73:ILE:HD13	1.75	0.67
2:C:1100:GLY:CA	3:D:458:LYS:HE3	2.24	0.67
12:C:1205:RFP:H402	12:C:1205:RFP:H313	1.77	0.67
2:C:476:PRO:O	3:D:856:ARG:NH2	2.27	0.67
3:D:106:TYR:HB3	3:D:312:MET:HE3	1.75	0.67
3:D:822:LEU:HD23	3:D:834:PRO:HA	1.77	0.67
2:C:169:GLN:OE1	2:C:370:ARG:NH2	2.26	0.67
3:D:155:MET:HE3	3:D:219:LEU:HB3	1.77	0.67
5:F:399:GLN:O	5:F:403:GLU:HG2	1.94	0.67
9:P:11:DA:H4'	9:P:12:DA:OP1	1.95	0.67
2:C:613:GLU:O	2:C:705:ALA:HB1	1.94	0.67
2:C:935:TRP:CB	2:C:982:SER:HB3	2.25	0.67
2:C:449:LEU:HB2	12:C:1205:RFP:H143	1.77	0.67
2:C:433:GLN:HE21	2:C:670:ASN:H	1.42	0.67
2:C:732:LEU:HA	2:C:737:VAL:CG1	2.24	0.67
1:A:152:ASN:CB	1:A:157:ALA:HB3	2.25	0.67
2:C:224:PRO:HB2	2:C:227:VAL:HG13	1.77	0.67
2:C:437:LEU:HB2	2:C:704:MET:CE	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:228:LEU:HD21	2:C:268:ILE:HG12	1.77	0.66
2:C:1034:ALA:HB2	3:D:447:MET:HG3	1.77	0.66
1:A:129:ASN:H	1:A:129:ASN:HD22	1.43	0.66
2:C:545:PHE:CD2	2:C:564:ALA:HB1	2.30	0.66
2:C:753:THR:HG21	2:C:799:PRO:HD2	1.78	0.66
8:O:19:DA:H4'	8:O:20:DT:OP1	1.95	0.66
1:A:63:PHE:HE1	2:C:741:ILE:HD13	1.61	0.66
2:C:375:LEU:HD13	2:C:427:LEU:HD22	1.76	0.66
2:C:872:ASP:N	2:C:872:ASP:OD1	2.17	0.66
3:D:1071:ASP:N	3:D:1072:GLY:HA2	2.09	0.66
3:D:139:VAL:CG1	3:D:231:PRO:HD3	2.26	0.66
3:D:74:ILE:HD12	7:J:42:VAL:HG13	1.77	0.66
2:C:102:ARG:HG2	2:C:125:PHE:HB2	1.78	0.66
3:D:931:ALA:O	3:D:932:ASN:ND2	2.28	0.66
4:E:57:ARG:NE	4:E:95:GLU:OE1	2.25	0.66
3:D:144:ARG:NH2	3:D:229:LEU:O	2.28	0.66
3:D:622:MET:CE	3:D:667:LEU:HD13	2.26	0.66
3:D:846:LEU:HD12	3:D:846:LEU:H	1.61	0.66
2:C:344:THR:O	2:C:355:PRO:HA	1.95	0.65
2:C:728:LEU:CD2	2:C:906:ILE:HG22	2.26	0.65
5:F:368:GLU:HG2	5:F:369:GLY:N	2.11	0.65
2:C:1116:LEU:O	2:C:1120:GLN:HG3	1.96	0.65
2:C:729:SER:OG	2:C:905:ASP:HA	1.97	0.65
2:C:1014:VAL:HG13	3:D:729:THR:HG21	1.78	0.65
1:A:56:ILE:HB	1:A:59:VAL:HG22	1.79	0.65
1:B:95:MET:HG2	1:B:113:PRO:CD	2.26	0.65
5:F:338:ALA:HB2	5:F:348:VAL:HG11	1.79	0.65
2:C:727:ILE:HG13	2:C:907:ILE:HB	1.79	0.65
3:D:17:ALA:O	3:D:21:ARG:HG3	1.97	0.65
1:B:29:GLY:HA2	1:B:190:ASP:OD2	1.96	0.65
2:C:984:LEU:CB	2:C:991:VAL:HG22	2.26	0.65
3:D:76:GLU:HA	7:J:44:PHE:HE2	1.61	0.65
1:A:108:GLY:CA	1:A:121:PRO:HB3	2.27	0.65
2:C:710:LEU:HD13	2:C:1021:ILE:HG12	1.79	0.65
2:C:584:MET:HA	2:C:619:THR:CG2	2.27	0.65
3:D:880:SER:O	3:D:995:GLY:HA3	1.97	0.64
2:C:728:LEU:HD22	2:C:906:ILE:HG22	1.79	0.64
2:C:899:PRO:HD2	2:C:992:MET:CE	2.27	0.64
3:D:886:ARG:HH12	14:D:2012:GLU:CA	2.11	0.64
5:F:180:ASN:OD1	5:F:183:GLU:HG3	1.96	0.64
1:A:66:VAL:HB	1:A:69:VAL:HG21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ILE:CG1	1:B:206:ASP:HB2	2.27	0.64
2:C:132:ASN:HB3	2:C:135:THR:CG2	2.28	0.64
2:C:429:GLN:OE1	2:C:442:HIS:NE2	2.30	0.64
2:C:509:LYS:O	2:C:516:THR:HG22	1.97	0.64
8:O:5:DG:H2"	8:O:6:DA:OP2	1.97	0.64
2:C:590:HIS:HB3	2:C:919:ILE:HD13	1.79	0.64
3:D:956:ILE:HD12	3:D:956:ILE:O	1.97	0.64
2:C:215:VAL:HG22	2:C:225:VAL:CA	2.28	0.64
2:C:718:GLU:H	3:D:724:THR:HG21	1.63	0.64
5:F:397:GLN:O	5:F:401:VAL:HG23	1.98	0.64
3:D:411:GLY:O	3:D:415:GLN:HB3	1.98	0.64
8:O:6:DA:C2'	8:O:7:DC:H5'	2.28	0.64
2:C:87:ILE:HD12	2:C:388:GLU:HG3	1.80	0.64
3:D:1086:ARG:HD2	3:D:1086:ARG:N	2.12	0.64
3:D:951:LEU:HD22	3:D:956:ILE:HG12	1.80	0.64
5:F:204:LEU:O	5:F:208:GLY:N	2.31	0.64
1:B:124:HIS:HE1	1:B:127:THR:HG23	1.63	0.64
2:C:203:LEU:HG	2:C:217:ILE:CG2	2.18	0.64
2:C:873:GLY:HA3	2:C:1028:VAL:HG11	1.80	0.64
3:D:799:ILE:CG2	3:D:803:LYS:HE2	2.28	0.64
1:B:147:VAL:HG13	1:B:166:SER:HB2	1.80	0.63
1:B:6:ARG:O	1:B:25:PRO:HD2	1.97	0.63
3:D:320:ILE:HG12	3:D:321:PRO:HD2	1.80	0.63
3:D:614:SER:HB2	3:D:615:PRO:HD2	1.79	0.63
3:D:673:ASN:HA	3:D:676:LEU:HD13	1.79	0.63
1:B:144:ARG:HB2	1:B:144:ARG:NH1	2.14	0.63
3:D:1081:LEU:CB	3:D:1113:MET:HE1	2.28	0.63
1:B:162:ILE:HG23	3:D:607:PRO:HG2	1.79	0.63
2:C:754:LYS:H	2:C:754:LYS:CE	2.11	0.63
3:D:155:MET:CE	3:D:219:LEU:HB3	2.28	0.63
3:D:468:ASN:ND2	5:F:463:ASP:OD2	2.32	0.63
3:D:799:ILE:HG21	3:D:803:LYS:HE2	1.80	0.63
5:F:191:ILE:O	5:F:195:LEU:HD13	1.97	0.63
2:C:534:GLN:HE21	2:C:534:GLN:HA	1.61	0.63
2:C:533:ALA:HB3	2:C:570:MET:HG3	1.81	0.63
3:D:1071:ASP:HB2	3:D:1072:GLY:C	2.19	0.63
4:E:29:PRO:HB2	4:E:33:THR:HG23	1.79	0.63
5:F:254:ALA:HA	10:F:502:SO4:O3	1.97	0.63
2:C:1043:ILE:HG23	2:C:1044:THR:H	1.64	0.63
2:C:338:ARG:HH11	2:C:343:GLN:HE22	1.44	0.63
2:C:751:ARG:NH1	3:D:332:GLY:O	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:661:TRP:CZ3	3:D:663:ALA:HB2	2.34	0.63
1:B:41:THR:O	1:B:45:SER:HB3	1.98	0.63
2:C:52:PHE:HZ	2:C:150:MET:HE2	1.63	0.63
3:D:781:THR:O	3:D:784:VAL:HG23	1.98	0.63
3:D:920:PHE:HE1	3:D:945:ASP:HA	1.62	0.63
1:A:42:LEU:O	1:A:171:VAL:HG11	1.98	0.63
2:C:727:ILE:HD12	2:C:907:ILE:HD12	1.81	0.63
3:D:1123:LEU:HA	3:D:1131:VAL:CG2	2.28	0.63
1:B:112:PRO:HB2	1:B:116:VAL:HG23	1.81	0.62
2:C:228:LEU:CD2	2:C:268:ILE:HG12	2.29	0.62
2:C:892:VAL:CG2	2:C:903:PRO:HG2	2.29	0.62
5:F:219:MET:HE2	5:F:219:MET:HA	1.81	0.62
1:A:9:LEU:HD23	1:B:221:LEU:O	1.98	0.62
2:C:1086:ASP:O	2:C:1090:ARG:HG2	1.99	0.62
2:C:560:GLU:HG3	2:C:561:PHE:H	1.63	0.62
3:D:1168:ILE:O	3:D:1178:PRO:HA	1.99	0.62
3:D:138:SER:HB3	3:D:253:THR:OG1	1.99	0.62
2:C:398:GLN:HB3	2:C:403:ILE:CG2	2.29	0.62
2:C:434:ASN:OD1	2:C:1025:HIS:ND1	2.31	0.62
3:D:444:PRO:HG3	3:D:521:ALA:O	1.99	0.62
3:D:642:PRO:HG3	3:D:661:TRP:CE2	2.35	0.62
5:F:402:LEU:HD23	5:F:414:ARG:HE	1.65	0.62
3:D:567:SER:HB3	3:D:574:LEU:HD13	1.81	0.62
2:C:393:GLU:OE2	5:F:247:ARG:HD3	2.00	0.62
2:C:132:ASN:CB	2:C:135:THR:HG22	2.28	0.62
2:C:783:ILE:HD13	2:C:784:GLY:N	2.15	0.62
3:D:430:ILE:HD13	3:D:541:MET:HG3	1.81	0.62
5:F:276:THR:HG23	7:J:89:ARG:NH2	2.15	0.62
1:B:72:ASP:OD1	1:B:73:VAL:N	2.27	0.62
3:D:52:PHE:O	3:D:91:ARG:HD2	2.00	0.62
2:C:193:VAL:CG1	2:C:205:PHE:HB2	2.29	0.62
2:C:87:ILE:O	2:C:95:SER:HA	2.00	0.62
9:P:11:DA:H2'	9:P:12:DA:C8	2.35	0.62
2:C:896:PRO:HB2	2:C:1001:LEU:HD13	1.82	0.62
3:D:648:ALA:O	3:D:652:GLU:HB2	2.00	0.62
3:D:665:THR:HG22	3:D:684:ASN:ND2	2.15	0.62
7:J:47:ASP:N	7:J:47:ASP:OD1	2.25	0.62
1:A:82:GLY:HA3	1:A:123:MET:HE1	1.80	0.62
2:C:742:HIS:HD2	2:C:868:ARG:HG3	1.64	0.62
3:D:1085:GLN:O	3:D:1086:ARG:O	2.18	0.62
3:D:587:TYR:O	3:D:590:THR:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1084:SER:OG	3:D:420:LYS:HD3	1.98	0.61
2:C:714:ILE:O	2:C:910:THR:OG1	2.18	0.61
1:A:211:ALA:O	1:A:215:LEU:N	2.33	0.61
2:C:128:ALA:HB1	2:C:405:PRO:HB3	1.80	0.61
2:C:641:ILE:HG21	2:C:644:VAL:HG13	1.80	0.61
3:D:666:THR:OG1	3:D:669:ARG:HG3	2.00	0.61
2:C:426:GLN:OE1	2:C:450:GLY:HA2	2.00	0.61
2:C:29:ARG:CD	2:C:964:ALA:HB2	2.30	0.61
3:D:12:ILE:HD11	3:D:1221:TRP:CE3	2.34	0.61
3:D:567:SER:HB3	3:D:574:LEU:CD1	2.30	0.61
3:D:64:LYS:NZ	3:D:76:GLU:OE2	2.32	0.61
4:E:29:PRO:HG2	4:E:34:ASN:HB2	1.80	0.61
3:D:706:ILE:O	3:D:710:GLN:HG3	2.01	0.61
3:D:755:ILE:HD12	3:D:776:ILE:CD1	2.25	0.61
3:D:755:ILE:CD1	3:D:776:ILE:HD11	2.27	0.61
2:C:1079:LEU:HD23	2:C:1083:LYS:HD2	1.82	0.61
3:D:460:LEU:HD11	3:D:472:ALA:CB	2.30	0.61
3:D:177:LEU:HD23	3:D:177:LEU:O	2.00	0.61
3:D:527:LEU:HD22	3:D:575:ALA:O	2.00	0.61
2:C:732:LEU:HA	2:C:737:VAL:HG12	1.83	0.61
2:C:593:ALA:HB2	3:D:852:THR:HG22	1.83	0.61
3:D:988:VAL:HG23	3:D:992:GLU:HG3	1.81	0.61
1:B:69:VAL:HG12	1:B:128:LEU:HA	1.81	0.61
3:D:622:MET:CE	3:D:629:VAL:HG22	2.31	0.61
5:F:181:ALA:O	5:F:185:VAL:HG23	2.00	0.61
1:B:76:ILE:HG23	1:B:125:ILE:CD1	2.31	0.61
2:C:729:SER:OG	2:C:904:VAL:O	2.19	0.61
2:C:575:ARG:NH2	2:C:966:PRO:HB2	2.15	0.60
2:C:764:ILE:HB	2:C:767:VAL:CG2	2.31	0.60
1:A:207:ALA:O	1:A:210:SER:OG	2.13	0.60
1:B:105:VAL:HG23	1:B:128:LEU:HD13	1.82	0.60
3:D:846:LEU:O	3:D:850:ILE:HG12	2.01	0.60
2:C:525:ASP:OD1	2:C:525:ASP:N	2.32	0.60
7:J:96:GLU:O	7:J:100:GLU:HG3	2.01	0.60
2:C:444:ARG:NH2	2:C:492:SER:O	2.34	0.60
2:C:900:ASP:OD2	2:C:992:MET:HG3	2.01	0.60
3:D:573:PRO:HG2	3:D:576:MET:CE	2.31	0.60
2:C:899:PRO:HD2	2:C:992:MET:HE1	1.83	0.60
2:C:946:TRP:CE2	2:C:978:GLY:HA3	2.36	0.60
3:D:889:ASP:OD2	3:D:891:GLU:N	2.35	0.60
3:D:886:ARG:NH1	14:D:2012:GLU:HB3	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:LEU:HD11	1:B:192:LEU:HD22	1.83	0.60
2:C:467:HIS:CG	2:C:468:PRO:HD2	2.37	0.60
2:C:498:ASN:OD1	2:C:499:PRO:HD2	2.01	0.60
2:C:533:ALA:HB2	2:C:567:VAL:HG11	1.84	0.60
2:C:932:LYS:HG2	2:C:1018:TYR:CE2	2.35	0.60
2:C:412:ARG:NH1	5:F:322:ARG:HH11	1.99	0.60
1:B:64:THR:O	1:B:65:THR:OG1	2.18	0.60
3:D:579:LEU:CD2	3:D:807:THR:HB	2.28	0.60
1:A:14:VAL:CG1	1:A:18:ARG:HG3	2.32	0.60
1:B:24:GLU:HG3	1:B:191:LYS:HG3	1.83	0.60
2:C:30:VAL:HG11	2:C:954:LEU:HG	1.84	0.60
3:D:505:HIS:CD2	3:D:1004:GLU:HG3	2.37	0.60
3:D:668:GLY:HA2	3:D:671:MET:HE3	1.82	0.60
1:A:24:GLU:OE1	1:A:191:LYS:HD3	2.02	0.60
2:C:404:THR:OG1	2:C:405:PRO:HD2	2.02	0.60
2:C:637:LYS:HD2	2:C:659:GLN:HE22	1.65	0.60
3:D:1121:GLU:OE2	3:D:1124:ARG:NH2	2.26	0.60
5:F:204:LEU:HD11	5:F:211:LEU:HD21	1.84	0.60
5:F:394:LEU:HB2	5:F:464:TYR:CE1	2.36	0.60
2:C:338:ARG:HH11	2:C:343:GLN:NE2	2.00	0.59
2:C:752:ASP:OD1	2:C:857:ASN:ND2	2.35	0.59
4:E:57:ARG:HH22	4:E:76:VAL:HG13	1.66	0.59
2:C:765:PRO:HD2	2:C:825:ASP:HB2	1.85	0.59
3:D:1249:LEU:HD12	3:D:1250:LYS:N	2.17	0.59
3:D:781:THR:CG2	3:D:814:ARG:HD2	2.31	0.59
5:F:274:ASP:OD1	7:J:89:ARG:NH2	2.25	0.59
5:F:462:ARG:NH1	5:F:465:LEU:HB2	2.17	0.59
3:D:1011:MET:CB	3:D:1029:LEU:HB2	2.32	0.59
3:D:287:GLN:CG	3:D:288:LYS:HZ2	2.16	0.59
5:F:308:VAL:HG21	8:O:23:DT:C7	2.27	0.59
1:A:9:LEU:HD13	1:A:23:ILE:CG1	2.31	0.59
2:C:622:GLU:HB3	2:C:703:GLU:HB2	1.84	0.59
3:D:435:GLN:OE1	3:D:435:GLN:N	2.31	0.59
3:D:550:GLU:O	3:D:554:GLU:HG3	2.02	0.59
1:A:14:VAL:HG12	1:A:19:SER:HA	1.84	0.59
1:B:102:PRO:HG3	1:B:131:LYS:H	1.66	0.59
1:B:144:ARG:HH11	1:B:144:ARG:HB2	1.65	0.59
3:D:1166:VAL:HA	3:D:1207:VAL:HG23	1.83	0.59
3:D:432:VAL:CG2	3:D:434:PRO:HD3	2.30	0.59
3:D:930:ASP:O	3:D:932:ASN:N	2.28	0.59
3:D:980:ARG:HD3	3:D:985:GLY:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ILE:HG23	1:B:125:ILE:HD11	1.85	0.59
5:F:444:ILE:O	5:F:448:THR:HG23	2.03	0.59
1:A:216:VAL:HG13	1:B:216:VAL:HG23	1.85	0.59
2:C:935:TRP:HB2	2:C:982:SER:CB	2.32	0.59
1:B:63:PHE:CZ	3:D:604:LYS:HG2	2.37	0.59
3:D:981:SER:HB3	3:D:984:THR:OG1	2.02	0.59
2:C:437:LEU:HB2	2:C:704:MET:HE1	1.85	0.59
5:F:234:LEU:HD23	5:F:270:VAL:HG21	1.84	0.59
1:B:158:GLU:HB3	1:B:161:ARG:HB2	1.84	0.59
2:C:876:LEU:HD11	2:C:886:ILE:HD11	1.83	0.59
3:D:193:VAL:O	3:D:197:VAL:HG23	2.03	0.59
1:B:162:ILE:CG2	3:D:607:PRO:HG2	2.33	0.59
3:D:58:TRP:CG	3:D:68:VAL:HG22	2.38	0.59
3:D:585:LEU:HD12	3:D:692:GLN:NE2	2.18	0.59
2:C:718:GLU:H	3:D:724:THR:CG2	2.16	0.59
1:A:2:LEU:HD12	1:B:143:GLY:HA2	1.84	0.58
1:B:183:VAL:HG22	3:D:488:GLU:OE2	2.03	0.58
1:B:22:VAL:HA	1:B:192:LEU:O	2.03	0.58
2:C:575:ARG:HE	2:C:967:VAL:HG22	1.67	0.58
3:D:937:ILE:CD1	3:D:951:LEU:HG	2.33	0.58
2:C:231:ALA:HB1	2:C:265:LEU:HD13	1.85	0.58
9:P:11:DA:H2"	9:P:12:DA:C5'	2.33	0.58
2:C:716:PRO:O	3:D:724:THR:HB	2.03	0.58
3:D:920:PHE:CE2	3:D:948:ILE:HG13	2.37	0.58
5:F:335:GLU:OE1	5:F:335:GLU:N	2.34	0.58
2:C:338:ARG:HB3	2:C:343:GLN:HG2	1.84	0.58
2:C:1028:VAL:HG12	3:D:429:VAL:CG1	2.34	0.58
3:D:656:LYS:N	3:D:656:LYS:HE3	2.08	0.58
3:D:656:LYS:HG2	3:D:656:LYS:O	2.03	0.58
2:C:545:PHE:HD2	2:C:564:ALA:HB1	1.67	0.58
3:D:1100:LEU:HD23	3:D:1101:SER:N	2.18	0.58
5:F:345:PRO:O	5:F:348:VAL:HG13	2.03	0.58
5:F:369:GLY:O	5:F:371:SER:N	2.37	0.58
1:A:33:THR:CG2	1:B:37:SER:HA	2.34	0.58
2:C:508:ARG:HD3	2:C:515:VAL:CG1	2.33	0.58
3:D:330:LEU:H	3:D:330:LEU:HD22	1.68	0.58
2:C:52:PHE:CZ	2:C:150:MET:HE2	2.39	0.58
2:C:380:ILE:HG12	2:C:418:ILE:HD11	1.86	0.58
3:D:1054:VAL:HG11	3:D:1100:LEU:HD21	1.86	0.58
3:D:238:GLU:O	3:D:238:GLU:HG3	2.02	0.58
3:D:505:HIS:HD2	3:D:1004:GLU:HG3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:573:SER:HB2	2:C:574:PRO:HD2	1.86	0.58
3:D:859:LEU:O	3:D:862:THR:HG22	2.03	0.58
4:E:57:ARG:HH12	4:E:76:VAL:HG12	1.69	0.58
1:A:42:LEU:O	1:A:46:ILE:HG12	2.04	0.57
2:C:771:VAL:HG23	2:C:792:ILE:CD1	2.34	0.57
3:D:527:LEU:HD21	3:D:581:MET:CE	2.34	0.57
7:J:68:ASP:HA	7:J:69:VAL:CB	2.22	0.57
1:B:212:GLY:O	1:B:216:VAL:HG12	2.05	0.57
2:C:578:VAL:HG13	2:C:582:THR:CB	2.33	0.57
2:C:636:ASP:N	2:C:636:ASP:OD1	2.34	0.57
1:A:40:ARG:HD3	1:B:33:THR:CG2	2.33	0.57
2:C:538:PRO:O	2:C:546:THR:HG23	2.04	0.57
3:D:116:TYR:HB3	3:D:298:VAL:HG11	1.86	0.57
3:D:656:LYS:CE	3:D:656:LYS:H	2.08	0.57
3:D:59:GLU:HG2	3:D:66:LYS:HG3	1.84	0.57
3:D:668:GLY:HA2	3:D:671:MET:CE	2.32	0.57
3:D:904:GLY:HA3	3:D:910:ILE:CG2	2.35	0.57
2:C:249:MET:O	2:C:253:LEU:HD23	2.05	0.57
3:D:737:VAL:HG13	3:D:738:PRO:HD2	1.87	0.57
2:C:590:HIS:O	2:C:919:ILE:HD11	2.04	0.57
2:C:732:LEU:CD2	2:C:737:VAL:HG11	2.34	0.57
3:D:137:THR:HG22	3:D:253:THR:O	2.04	0.57
3:D:1266:SER:H	14:D:2012:GLU:N	2.03	0.57
3:D:20:ILE:HD13	3:D:318:PRO:HD3	1.85	0.57
1:B:151:GLN:OE1	1:B:151:GLN:N	2.30	0.57
2:C:106:VAL:HG11	2:C:120:TYR:CE1	2.39	0.57
2:C:348:VAL:HB	2:C:349:PRO:CD	2.28	0.57
2:C:809:GLU:O	2:C:813:ARG:HG2	2.05	0.57
3:D:693:ALA:O	3:D:697:ASN:HB2	2.05	0.57
3:D:920:PHE:CE1	3:D:945:ASP:HA	2.40	0.57
4:E:57:ARG:HD3	4:E:57:ARG:O	2.04	0.57
1:A:21:PHE:HB2	1:A:194:ILE:HG12	1.87	0.57
1:B:76:ILE:HA	1:B:79:ASN:HB2	1.85	0.57
2:C:128:ALA:CB	2:C:405:PRO:HB3	2.35	0.57
2:C:622:GLU:OE1	2:C:622:GLU:N	2.38	0.57
3:D:218:ARG:O	3:D:222:ILE:HG13	2.04	0.57
4:E:85:GLN:H	4:E:85:GLN:NE2	2.02	0.57
2:C:481:GLU:O	2:C:485:ILE:HD11	2.05	0.57
2:C:477:ILE:CD1	3:D:852:THR:HG21	2.34	0.57
2:C:412:ARG:HD2	5:F:322:ARG:NE	2.19	0.57
1:B:32:TYR:CE2	1:B:178:VAL:HG21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1048:LEU:O	2:C:1055:GLY:HA3	2.05	0.56
2:C:231:ALA:HB1	2:C:265:LEU:CD1	2.34	0.56
2:C:299:LEU:CB	2:C:323:THR:HB	2.35	0.56
2:C:710:LEU:O	2:C:1018:TYR:HA	2.04	0.56
3:D:1037:GLU:HG2	3:D:1039:ARG:NH1	2.20	0.56
3:D:785:GLY:O	3:D:789:GLU:HG3	2.04	0.56
1:B:102:PRO:HB3	1:B:130:ASP:HA	1.87	0.56
1:B:22:VAL:HG12	1:B:193:ILE:HD12	1.87	0.56
2:C:748:ILE:HD11	2:C:796:LYS:NZ	2.20	0.56
3:D:1168:ILE:HD11	3:D:1182:THR:HG21	1.86	0.56
3:D:240:LEU:HD23	3:D:244:LEU:HG	1.88	0.56
5:F:166:VAL:O	5:F:170:LEU:HG	2.05	0.56
5:F:423:GLN:O	5:F:423:GLN:HG3	2.05	0.56
8:O:11:DA:H2"	8:O:12:DG:H5"	1.88	0.56
1:A:33:THR:HG21	1:B:37:SER:HA	1.88	0.56
1:A:210:SER:HB3	1:B:229:SER:HB3	1.87	0.56
2:C:432:ASP:HB2	12:C:1205:RFP:H20C	1.86	0.56
2:C:892:VAL:HG22	2:C:903:PRO:HG2	1.86	0.56
2:C:1072:ALA:HB1	3:D:554:GLU:OE2	2.04	0.56
7:J:106:LYS:O	7:J:108:LYS:HG3	2.05	0.56
2:C:710:LEU:CD2	2:C:1021:ILE:HD11	2.26	0.56
2:C:262:ASP:OD2	2:C:280:LYS:HE2	2.05	0.56
2:C:534:GLN:NE2	2:C:534:GLN:HA	2.21	0.56
3:D:665:THR:HG21	3:D:682:PHE:CE2	2.41	0.56
5:F:272:LYS:HE3	8:O:25:DC:OP1	2.05	0.56
1:B:85:VAL:HG23	1:B:117:THR:C	2.26	0.56
2:C:776:ASP:HB2	2:C:777:GLU:OE1	2.05	0.56
2:C:805:LEU:H	2:C:805:LEU:HD22	1.70	0.56
3:D:106:TYR:HB3	3:D:312:MET:CE	2.34	0.56
3:D:130:TYR:O	3:D:372:ARG:HD3	2.06	0.56
3:D:281:ILE:HG22	3:D:289:LYS:HG3	1.86	0.56
3:D:460:LEU:HD11	3:D:472:ALA:HB1	1.87	0.56
3:D:884:ILE:HD12	3:D:885:VAL:O	2.05	0.56
3:D:957:THR:O	3:D:958:THR:HG23	2.05	0.56
1:A:39:ARG:O	1:A:43:LEU:HD13	2.05	0.56
1:B:143:GLY:HA3	1:B:168:TYR:CD1	2.41	0.56
1:B:180:ALA:HA	1:B:189:PHE:O	2.05	0.56
2:C:698:CYS:O	2:C:705:ALA:N	2.30	0.56
5:F:180:ASN:OD1	5:F:182:GLU:HG2	2.06	0.56
1:A:66:VAL:HB	1:A:69:VAL:CG2	2.36	0.56
1:B:147:VAL:CG1	1:B:166:SER:HB2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:229:LEU:HD11	2:C:234:TRP:CE3	2.41	0.56
2:C:899:PRO:CD	2:C:992:MET:HE1	2.36	0.56
3:D:274:ALA:O	3:D:278:ARG:HG2	2.06	0.56
3:D:708:VAL:O	3:D:712:VAL:HG23	2.06	0.56
7:J:74:LYS:O	7:J:74:LYS:HD3	2.06	0.56
1:A:8:THR:O	1:A:23:ILE:HA	2.06	0.56
1:B:2:LEU:CB	1:B:231:HIS:HA	2.36	0.56
2:C:269:TYR:CE2	2:C:278:PRO:HB3	2.41	0.56
2:C:523:THR:HG23	2:C:526:GLU:CD	2.25	0.56
3:D:1088:ARG:HG2	3:D:1089:VAL:N	2.16	0.56
3:D:1276:THR:CG2	4:E:102:GLU:HG3	2.34	0.56
1:B:95:MET:CB	1:B:110:ILE:HD11	2.36	0.56
2:C:556:GLY:N	2:C:557:GLY:HA2	2.21	0.56
3:D:31:PRO:HB2	3:D:345:ARG:HG2	1.86	0.56
1:B:63:PHE:CD1	3:D:604:LYS:HA	2.41	0.56
3:D:588:LEU:HD22	3:D:668:GLY:CA	2.35	0.56
2:C:714:ILE:HG22	2:C:714:ILE:O	2.06	0.55
3:D:58:TRP:HZ3	3:D:71:LYS:HB2	1.70	0.55
4:E:85:GLN:H	4:E:85:GLN:HE21	1.54	0.55
1:A:40:ARG:HH11	1:B:33:THR:CG2	2.19	0.55
2:C:1011:PRO:HB2	2:C:1012:TYR:CD2	2.41	0.55
2:C:204:GLU:O	2:C:216:ARG:N	2.38	0.55
2:C:215:VAL:N	2:C:223:GLN:O	2.40	0.55
2:C:598:MET:O	2:C:602:MET:HG3	2.06	0.55
2:C:623:LEU:H	2:C:623:LEU:HD12	1.70	0.55
3:D:103:HIS:CE1	3:D:105:TRP:HB2	2.41	0.55
3:D:930:ASP:OD1	3:D:934:ASN:HB2	2.06	0.55
5:F:359:ILE:HG22	5:F:360:SER:H	1.70	0.55
8:O:16:DT:H6	8:O:16:DT:H5'	1.71	0.55
1:B:21:PHE:HB2	1:B:194:ILE:HG22	1.88	0.55
1:B:94:THR:HA	1:B:138:LEU:O	2.05	0.55
2:C:186:THR:HG23	2:C:188:LYS:H	1.72	0.55
2:C:265:LEU:HD11	2:C:287:LEU:HG	1.87	0.55
1:A:70:LYS:NZ	2:C:682:ASP:OD1	2.38	0.55
2:C:704:MET:CE	2:C:706:LEU:HD21	2.37	0.55
3:D:1229:GLU:O	3:D:1233:VAL:HG23	2.06	0.55
1:B:74:THR:HG21	3:D:608:GLU:OE1	2.06	0.55
8:O:14:DG:C8	8:O:15:DT:H72	2.41	0.55
8:O:6:DA:H1'	8:O:7:DC:H5'	1.88	0.55
2:C:280:LYS:HB3	2:C:280:LYS:NZ	2.21	0.55
2:C:328:ASP:O	2:C:332:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:509:LYS:HA	2:C:569:TYR:HA	1.87	0.55
3:D:1181:LEU:CD1	3:D:1213:LYS:HE2	2.36	0.55
3:D:448:ALA:HB1	3:D:491:ILE:HD11	1.88	0.55
3:D:468:ASN:OD1	3:D:470:LYS:HB2	2.06	0.55
3:D:872:LEU:HG	3:D:876:LEU:CD2	2.37	0.55
3:D:924:LEU:HD21	3:D:959:VAL:CG1	2.36	0.55
2:C:1068:GLN:NE2	3:D:1249:LEU:HD13	2.22	0.55
2:C:167:VAL:HG13	2:C:445:ARG:O	2.07	0.55
2:C:935:TRP:HA	2:C:983:THR:HG23	1.89	0.55
2:C:984:LEU:HD13	2:C:991:VAL:CG2	2.33	0.55
3:D:190:LYS:HZ2	3:D:192:ASP:HB3	1.69	0.55
3:D:237:ASP:HB3	3:D:240:LEU:HB3	1.88	0.55
3:D:70:PHE:O	3:D:82:VAL:HG11	2.07	0.55
5:F:321:GLN:O	5:F:325:LEU:HB2	2.07	0.55
5:F:430:ILE:O	5:F:433:VAL:HG13	2.06	0.55
1:A:193:ILE:O	1:A:193:ILE:HD12	2.07	0.55
2:C:233:GLY:HA2	2:C:261:THR:CB	2.37	0.55
3:D:190:LYS:HD2	3:D:192:ASP:H	1.71	0.55
3:D:740:GLN:H	3:D:740:GLN:HE21	1.54	0.55
1:B:93:VAL:HG11	1:B:116:VAL:HG11	1.87	0.55
2:C:437:LEU:HB2	2:C:704:MET:HE2	1.89	0.55
2:C:578:VAL:HG12	2:C:579:SER:O	2.07	0.55
2:C:583:ALA:O	2:C:619:THR:HG21	2.06	0.55
1:A:177:LYS:HG2	1:A:193:ILE:HD11	1.89	0.55
1:B:39:ARG:O	1:B:43:LEU:HB2	2.07	0.55
2:C:1035:ARG:CZ	2:C:1047:PRO:HB3	2.37	0.55
2:C:227:VAL:HG23	2:C:268:ILE:HD11	1.88	0.55
3:D:1071:ASP:N	3:D:1071:ASP:OD2	2.40	0.55
3:D:704:PRO:HD2	3:D:707:VAL:HG21	1.89	0.55
3:D:923:THR:O	3:D:961:VAL:HG23	2.06	0.55
5:F:219:MET:HA	5:F:219:MET:CE	2.37	0.55
2:C:921:GLN:HB2	2:C:1019:MET:CE	2.36	0.54
3:D:910:ILE:HG23	3:D:910:ILE:O	2.07	0.54
2:C:1026:HIS:HB3	2:C:1031:LYS:HE3	1.88	0.54
2:C:45:LEU:CD2	2:C:443:LYS:HD2	2.38	0.54
3:D:1089:VAL:HG13	3:D:1098:GLY:C	2.28	0.54
3:D:912:ASP:OD1	3:D:913:ALA:N	2.40	0.54
5:F:320:ILE:O	5:F:324:LEU:HB2	2.07	0.54
2:C:102:ARG:CG	2:C:125:PHE:HB2	2.38	0.54
2:C:454:LEU:HD22	2:C:459:ALA:CB	2.37	0.54
2:C:789:ASP:HA	2:C:830:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:527:LEU:CD1	3:D:712:VAL:HG12	2.37	0.54
3:D:747:ARG:O	3:D:751:GLU:HG3	2.08	0.54
3:D:962:ARG:HB3	3:D:977:CYS:HA	1.89	0.54
2:C:1028:VAL:HG12	3:D:429:VAL:HG12	1.88	0.54
3:D:1034:GLU:OE2	3:D:1041:PRO:HA	2.06	0.54
2:C:324:LEU:O	2:C:325:THR:O	2.25	0.54
2:C:338:ARG:NH1	2:C:343:GLN:HE22	2.05	0.54
2:C:435:ASN:HB2	2:C:436:PRO:HD2	1.90	0.54
3:D:951:LEU:CB	3:D:956:ILE:HD11	2.27	0.54
9:P:11:DA:H2'	9:P:12:DA:H8	1.70	0.54
2:C:560:GLU:OE1	2:C:560:GLU:HA	2.08	0.54
2:C:614:ALA:HB1	2:C:615:PRO:HD2	1.89	0.54
2:C:736:ASP:OD1	2:C:869:LYS:HE2	2.08	0.54
3:D:334:ARG:HD3	5:F:356:ARG:HH21	1.72	0.54
4:E:81:GLU:OE1	4:E:81:GLU:HA	2.07	0.54
2:C:412:ARG:HD2	5:F:322:ARG:HE	1.73	0.54
7:J:79:ARG:NH2	8:O:25:DC:OP1	2.41	0.54
1:A:34:LEU:HD11	1:B:218:LEU:HD13	1.90	0.54
1:B:63:PHE:CE2	3:D:603:THR:HG23	2.43	0.54
2:C:727:ILE:CG1	2:C:907:ILE:HB	2.38	0.54
3:D:878:ASP:OD1	3:D:1215:SER:HB2	2.07	0.54
3:D:226:PHE:CE1	3:D:248:TYR:HB3	2.43	0.54
3:D:740:GLN:O	3:D:744:ILE:HG13	2.08	0.54
1:A:63:PHE:CE1	2:C:741:ILE:HD13	2.41	0.54
1:B:20:ARG:HG2	1:B:195:ASP:OD1	2.08	0.54
2:C:221:ARG:HG3	2:C:222:ARG:HG3	1.90	0.54
2:C:1126:VAL:HG12	3:D:12:ILE:HG23	1.90	0.54
3:D:336:ALA:HA	5:F:359:ILE:O	2.08	0.54
3:D:661:TRP:HZ3	3:D:663:ALA:HB2	1.73	0.54
2:C:477:ILE:HD11	3:D:852:THR:HG21	1.90	0.54
3:D:924:LEU:HD22	3:D:926:THR:O	2.08	0.54
5:F:385:ALA:O	5:F:389:VAL:HG23	2.08	0.54
3:D:67:ARG:NH1	5:F:423:GLN:HA	2.23	0.54
1:A:82:GLY:HA3	1:A:123:MET:CE	2.37	0.54
2:C:652:MET:HE2	2:C:658:ARG:HD2	1.89	0.54
3:D:1071:ASP:HB2	3:D:1072:GLY:CA	2.38	0.54
3:D:1251:GLU:OE1	3:D:1251:GLU:N	2.37	0.54
1:A:34:LEU:HD11	1:B:218:LEU:CD1	2.38	0.53
1:A:98:ARG:O	1:A:99:LYS:HD2	2.08	0.53
3:D:1168:ILE:HD13	3:D:1176:PHE:CB	2.36	0.53
3:D:599:TYR:HA	3:D:610:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:86:GLU:OE1	4:E:91:ILE:HG12	2.07	0.53
5:F:194:GLY:HA2	5:F:222:ILE:HG22	1.90	0.53
1:A:68:GLY:CA	1:A:129:ASN:HD21	2.21	0.53
1:A:211:ALA:O	1:A:215:LEU:HB2	2.08	0.53
1:B:198:THR:HG21	1:B:202:ILE:HG23	1.90	0.53
2:C:178:PHE:HD1	2:C:193:VAL:HB	1.73	0.53
2:C:338:ARG:HB3	2:C:343:GLN:CG	2.37	0.53
2:C:510:VAL:HG11	2:C:567:VAL:HG12	1.90	0.53
2:C:911:HIS:CE1	3:D:579:LEU:O	2.61	0.53
3:D:799:ILE:HG23	3:D:803:LYS:HG3	1.90	0.53
3:D:269:ASP:OD2	3:D:272:ALA:N	2.40	0.53
2:C:754:LYS:HD3	3:D:39:LEU:CD1	2.38	0.53
1:T:260:SER:O	1:T:264:LEU:HG	2.08	0.53
1:A:18:ARG:HB2	1:A:196:VAL:O	2.09	0.53
2:C:676:ASN:OD1	2:C:677:GLN:N	2.41	0.53
1:A:71:GLU:OE2	1:A:126:ALA:HA	2.08	0.53
1:B:95:MET:HB2	1:B:110:ILE:HD11	1.89	0.53
2:C:114:LYS:HG2	2:C:161:GLY:O	2.09	0.53
5:F:306:ILE:CG2	5:F:310:MET:HB3	2.39	0.53
5:F:404:THR:OG1	5:F:457:ARG:NE	2.41	0.53
1:A:177:LYS:CE	1:A:193:ILE:HD11	2.27	0.53
1:A:219:PHE:CE1	1:B:215:LEU:HD13	2.44	0.53
2:C:250:MET:HA	2:C:253:LEU:HD21	1.89	0.53
2:C:272:LEU:C	2:C:274:PRO:HD3	2.29	0.53
2:C:510:VAL:HG23	2:C:514:VAL:C	2.29	0.53
2:C:538:PRO:HB2	2:C:546:THR:OG1	2.07	0.53
2:C:481:GLU:HG2	2:C:597:LEU:CD2	2.38	0.53
5:F:164:ASP:OD1	5:F:166:VAL:HG22	2.09	0.53
3:D:354:LEU:O	3:D:358:ILE:HG12	2.09	0.53
1:B:183:VAL:HG13	3:D:488:GLU:OE2	2.09	0.53
3:D:498:LEU:HD11	3:D:543:VAL:HG22	1.91	0.53
1:B:63:PHE:CE1	3:D:604:LYS:HA	2.44	0.53
2:C:1117:LYS:HE2	3:D:90:GLU:O	2.09	0.53
2:C:45:LEU:HD22	2:C:443:LYS:HD2	1.91	0.53
2:C:751:ARG:HG2	2:C:856:VAL:HG22	1.89	0.53
3:D:498:LEU:CD1	3:D:543:VAL:HG22	2.39	0.53
2:C:910:THR:CG2	3:D:730:VAL:HG23	2.37	0.53
2:C:144:PHE:O	2:C:411:ILE:HD13	2.09	0.53
3:D:26:GLY:HA3	3:D:51:ILE:HG23	1.91	0.53
3:D:844:THR:H	3:D:847:GLU:HB2	1.74	0.53
5:F:241:VAL:HG22	5:F:289:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1001:LEU:HD21	2:C:1016:VAL:HG11	1.91	0.53
2:C:412:ARG:NH1	5:F:322:ARG:NH1	2.57	0.53
3:D:6:PHE:CD1	3:D:1257:LYS:HE3	2.44	0.53
3:D:1275:PRO:HG3	4:E:76:VAL:CG1	2.39	0.53
3:D:759:TYR:CE1	3:D:766:HIS:HA	2.44	0.53
5:F:272:LYS:HB2	7:J:84:MET:CE	2.39	0.53
1:A:108:GLY:HA2	1:A:121:PRO:HB3	1.90	0.52
1:B:84:VAL:HB	1:B:199:LYS:CD	2.37	0.52
3:D:66:LYS:O	3:D:66:LYS:HG2	2.08	0.52
3:D:745:LEU:O	3:D:749:GLU:HG2	2.08	0.52
3:D:850:ILE:O	3:D:853:HIS:HB2	2.09	0.52
1:A:40:ARG:NH1	1:B:33:THR:CG2	2.69	0.52
1:B:68:GLY:O	1:B:129:ASN:N	2.39	0.52
2:C:510:VAL:HG12	2:C:568:ASP:C	2.29	0.52
3:D:1153:LYS:O	3:D:1157:VAL:HG23	2.09	0.52
3:D:737:VAL:CG1	3:D:738:PRO:HD2	2.39	0.52
3:D:741:LYS:NZ	3:D:818:GLY:O	2.42	0.52
3:D:927:ASP:HB3	3:D:935:VAL:HG11	1.91	0.52
5:F:170:LEU:HA	5:F:173:ILE:HG12	1.90	0.52
8:O:16:DT:C6	8:O:16:DT:H5'	2.44	0.52
1:A:30:PHE:CE1	1:B:40:ARG:HG3	2.44	0.52
2:C:911:HIS:O	2:C:914:PRO:HD2	2.09	0.52
3:D:1088:ARG:HA	3:D:1114:GLU:OE1	2.08	0.52
3:D:1088:ARG:HD2	3:D:1111:GLN:HB3	1.90	0.52
3:D:287:GLN:HG2	3:D:288:LYS:HZ2	1.75	0.52
5:F:272:LYS:HE2	7:J:84:MET:HE2	1.92	0.52
2:C:1041:SER:HB3	2:C:1044:THR:O	2.09	0.52
2:C:613:GLU:HB3	2:C:708:LYS:HD3	1.91	0.52
2:C:766:ASN:HB3	5:F:465:LEU:HD21	1.90	0.52
3:D:890:CYS:SG	3:D:892:THR:HG22	2.49	0.52
4:E:35:PRO:HG2	4:E:40:LEU:HD11	1.91	0.52
1:B:124:HIS:CE1	1:B:127:THR:HG23	2.45	0.52
1:B:151:GLN:HG2	1:B:151:GLN:O	2.09	0.52
2:C:729:SER:HA	2:C:895:MET:CE	2.38	0.52
3:D:1128:PRO:HG3	3:D:1206:PRO:CB	2.39	0.52
3:D:139:VAL:O	15:D:2101:HOH:O	2.19	0.52
1:B:202:ILE:HG12	1:B:206:ASP:HB2	1.91	0.52
2:C:33:ALA:HB2	2:C:966:PRO:HG3	1.92	0.52
2:C:449:LEU:N	2:C:449:LEU:HD12	2.25	0.52
3:D:28:VAL:HG11	3:D:319:VAL:HG21	1.92	0.52
3:D:873:THR:O	3:D:877:VAL:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:234:LEU:CD2	5:F:270:VAL:HG21	2.39	0.52
5:F:359:ILE:HG22	5:F:360:SER:N	2.24	0.52
9:P:3:DC:H2''	9:P:4:DA:C8	2.45	0.52
1:A:22:VAL:HG23	1:A:193:ILE:HG22	1.92	0.52
2:C:1028:VAL:O	2:C:1032:ILE:HG22	2.09	0.52
2:C:560:GLU:CG	2:C:561:PHE:H	2.22	0.52
3:D:73:ILE:HD12	7:J:45:ALA:HB2	1.90	0.52
3:D:91:ARG:O	3:D:321:PRO:HG3	2.10	0.52
9:P:17:DT:O5'	1:T:290:GLY:HA3	2.09	0.52
1:A:14:VAL:HG13	1:A:15:ALA:H	1.74	0.52
1:A:70:LYS:HD3	1:A:127:THR:HG21	1.92	0.52
2:C:239:ILE:CG2	2:C:253:LEU:HD22	2.40	0.52
3:D:881:GLN:HE22	3:D:1250:LYS:HE2	1.75	0.52
3:D:271:ASP:HA	3:D:303:GLN:NE2	2.23	0.52
3:D:631:ALA:O	3:D:666:THR:HA	2.10	0.52
3:D:676:LEU:HD12	3:D:676:LEU:N	2.25	0.52
5:F:201:LEU:HD11	5:F:219:MET:CB	2.40	0.52
5:F:174:GLY:HA2	5:F:239:ARG:CZ	2.40	0.52
5:F:290:ARG:HH11	11:F:506:EDO:H22	1.74	0.52
1:A:11:GLU:OE1	1:A:205:ARG:NE	2.43	0.52
2:C:269:TYR:CD2	2:C:278:PRO:HB3	2.45	0.52
2:C:398:GLN:HB3	2:C:403:ILE:HG22	1.92	0.52
3:D:1037:GLU:OE2	3:D:1212:THR:HB	2.09	0.52
3:D:1056:LEU:HD21	3:D:1063:PHE:CD1	2.45	0.52
3:D:47:PHE:CD1	3:D:322:PRO:HB3	2.44	0.52
3:D:585:LEU:HD12	3:D:692:GLN:HE21	1.75	0.52
5:F:290:ARG:NH1	11:F:506:EDO:C1	2.73	0.52
5:F:293:ILE:O	5:F:297:MET:HG3	2.09	0.52
1:A:9:LEU:HD23	1:B:221:LEU:C	2.30	0.52
12:C:1205:RFP:HC43	12:C:1205:RFP:O11	2.10	0.52
2:C:174:PRO:HA	2:C:196:ILE:HG23	1.92	0.52
3:D:365:ILE:HD13	5:F:235:GLU:HG2	1.91	0.52
5:F:313:VAL:CG2	5:F:351:ILE:HD13	2.40	0.52
7:J:31:ARG:HG2	7:J:41:ASP:OD1	2.10	0.52
8:O:1:DG:H2''	8:O:2:DC:H5'	1.92	0.52
2:C:496:ARG:HH21	2:C:521:TYR:CB	2.23	0.51
2:C:720:HIS:O	3:D:432:VAL:HG11	2.10	0.51
2:C:754:LYS:HD3	3:D:39:LEU:HD12	1.92	0.51
2:C:508:ARG:HH11	2:C:570:MET:HE2	1.74	0.51
3:D:630:ARG:HH11	11:D:2011:EDO:H21	1.76	0.51
3:D:740:GLN:H	3:D:740:GLN:NE2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:P:17:DT:H5''	1:T:290:GLY:N	2.25	0.51
1:A:99:LYS:HE3	1:A:109:ASP:OD1	2.09	0.51
2:C:1031:LYS:NZ	10:C:1203:SO4:S	2.83	0.51
2:C:1078:GLU:OE2	3:D:547:LEU:HB2	2.11	0.51
2:C:652:MET:CE	2:C:658:ARG:HD2	2.40	0.51
2:C:849:ASP:O	2:C:850:ASP:O	2.28	0.51
7:J:58:ASN:HD21	7:J:60:LEU:HD12	1.76	0.51
7:J:90:SER:N	7:J:93:GLU:OE1	2.36	0.51
2:C:176:VAL:HG13	2:C:307:VAL:HG11	1.92	0.51
2:C:148:PHE:HE1	2:C:380:ILE:HD11	1.75	0.51
2:C:578:VAL:HG13	2:C:582:THR:CG2	2.41	0.51
2:C:771:VAL:HG22	2:C:772:LEU:CD1	2.23	0.51
3:D:137:THR:HG22	3:D:253:THR:C	2.30	0.51
2:C:911:HIS:ND1	3:D:579:LEU:O	2.43	0.51
3:D:642:PRO:HD3	3:D:656:LYS:CD	2.34	0.51
3:D:739:PRO:HD3	3:D:791:PHE:CE2	2.45	0.51
3:D:73:ILE:HG12	3:D:82:VAL:HG11	1.92	0.51
5:F:317:LEU:HD23	5:F:317:LEU:O	2.10	0.51
5:F:465:LEU:O	5:F:466:ASP:HB2	2.10	0.51
1:B:28:PRO:HD3	1:B:189:PHE:CD1	2.46	0.51
3:D:1119:PRO:HA	3:D:1122:VAL:CG1	2.40	0.51
3:D:1122:VAL:HG23	3:D:1126:GLN:NE2	2.24	0.51
3:D:579:LEU:HA	3:D:806:ALA:HB1	1.93	0.51
2:C:973:GLU:CA	3:D:732:MET:HE3	2.40	0.51
3:D:930:ASP:OD2	3:D:931:ALA:N	2.44	0.51
5:F:289:ILE:O	5:F:293:ILE:HG13	2.10	0.51
7:J:28:GLN:HG2	7:J:46:ASP:HA	1.91	0.51
8:O:15:DT:H6	8:O:15:DT:OP2	1.93	0.51
2:C:433:GLN:CG	2:C:670:ASN:HB2	2.41	0.51
3:D:735:VAL:O	3:D:840:ARG:NE	2.39	0.51
8:O:12:DG:H2''	8:O:13:DT:C5'	2.41	0.51
8:O:15:DT:H2''	8:O:16:DT:OP2	2.11	0.51
2:C:151:MET:SD	2:C:155:GLY:HA2	2.50	0.51
2:C:797:VAL:CG1	2:C:823:VAL:HB	2.40	0.51
2:C:796:LYS:HB3	2:C:826:THR:O	2.10	0.51
2:C:747:GLU:HG3	2:C:859:LEU:HD21	1.91	0.51
3:D:1191:ASN:OD1	3:D:1202:ALA:HB3	2.11	0.51
3:D:225:THR:HG21	3:D:244:LEU:HD11	1.93	0.51
3:D:590:THR:HG23	3:D:630:ARG:HE	1.75	0.51
3:D:687:MET:HE2	3:D:695:ILE:CD1	2.41	0.51
5:F:338:ALA:HB1	5:F:343:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:394:LEU:HB2	5:F:464:TYR:CD1	2.46	0.51
7:J:50:ILE:HG22	7:J:64:LEU:HD11	1.93	0.51
1:A:147:VAL:HG12	1:A:168:TYR:HE2	1.76	0.51
1:A:219:PHE:HE1	1:B:38:LEU:HD21	1.75	0.51
2:C:1086:ASP:OD1	2:C:1107:GLY:N	2.41	0.51
3:D:43:LYS:O	3:D:44:ASP:HB2	2.11	0.51
3:D:641:ARG:O	3:D:682:PHE:HB2	2.11	0.51
1:A:27:GLU:OE2	1:B:144:ARG:NH2	2.44	0.50
1:B:33:THR:OG1	1:B:34:LEU:N	2.43	0.50
1:A:138:LEU:HD12	1:A:138:LEU:N	2.26	0.50
2:C:215:VAL:HG23	2:C:223:GLN:CB	2.41	0.50
2:C:965:THR:O	2:C:965:THR:OG1	2.25	0.50
3:D:642:PRO:HG3	3:D:661:TRP:CD2	2.46	0.50
3:D:738:PRO:HA	3:D:791:PHE:HD2	1.76	0.50
1:B:105:VAL:HG12	1:B:125:ILE:HG21	1.93	0.50
1:B:60:LEU:HD22	1:B:60:LEU:N	2.26	0.50
2:C:196:ILE:HG23	2:C:196:ILE:O	2.11	0.50
2:C:712:VAL:CG1	2:C:925:THR:HG23	2.41	0.50
3:D:249:GLY:HA2	3:D:252:PHE:CE2	2.47	0.50
1:A:36:ASN:CB	2:C:1007:GLY:HA3	2.41	0.50
3:D:444:PRO:HD2	3:D:447:MET:CE	2.41	0.50
3:D:951:LEU:C	3:D:956:ILE:HD11	2.31	0.50
7:J:97:LEU:HD23	7:J:97:LEU:O	2.11	0.50
1:T:264:LEU:HB3	1:T:269:VAL:HG21	1.92	0.50
1:B:30:PHE:HA	1:B:33:THR:HG23	1.92	0.50
1:B:85:VAL:HG23	1:B:117:THR:O	2.12	0.50
2:C:372:VAL:O	2:C:376:ILE:HG12	2.12	0.50
2:C:639:GLY:HA3	2:C:653:ALA:HA	1.92	0.50
2:C:638:THR:HG23	2:C:688:GLU:HA	1.91	0.50
2:C:910:THR:O	2:C:914:PRO:HD3	2.12	0.50
2:C:931:ALA:HB1	2:C:961:SER:O	2.11	0.50
5:F:164:ASP:OD1	5:F:165:SER:N	2.44	0.50
2:C:199:ARG:NH2	2:C:295:LYS:O	2.40	0.50
2:C:29:ARG:HG2	2:C:964:ALA:HB2	1.93	0.50
3:D:118:LEU:HB2	3:D:120:LEU:HD13	1.93	0.50
5:F:254:ALA:HB3	5:F:257:ASP:OD2	2.11	0.50
8:O:1:DG:H2''	8:O:2:DC:C5'	2.41	0.50
1:A:79:ASN:O	1:A:123:MET:HE1	2.11	0.50
1:A:214:THR:HG23	1:B:231:HIS:CG	2.47	0.50
2:C:898:LEU:HD23	2:C:1001:LEU:CD2	2.42	0.50
2:C:169:GLN:HB2	2:C:427:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:726:ILE:O	2:C:887:GLY:N	2.41	0.50
2:C:913:VAL:HB	2:C:914:PRO:HD3	1.93	0.50
1:A:5:GLN:HG3	1:A:25:PRO:CG	2.42	0.50
2:C:215:VAL:HG23	2:C:223:GLN:HB3	1.94	0.50
2:C:139:LYS:NZ	2:C:401:GLU:O	2.45	0.50
3:D:1081:LEU:HB3	3:D:1113:MET:CE	2.42	0.50
1:B:172:LEU:HD12	3:D:620:MET:SD	2.52	0.50
3:D:656:LYS:HB2	3:D:659:ASP:O	2.12	0.50
1:B:44:SER:HA	1:B:145:GLY:HA2	1.92	0.50
2:C:239:ILE:HG21	2:C:253:LEU:HD22	1.93	0.50
3:D:269:ASP:HB3	3:D:272:ALA:HB3	1.93	0.50
3:D:463:LEU:HB2	3:D:465:HIS:HD2	1.77	0.50
3:D:848:TYR:O	3:D:852:THR:HG23	2.12	0.50
1:A:119:HIS:CD2	1:A:201:SER:HA	2.47	0.49
2:C:132:ASN:O	2:C:136:GLY:N	2.43	0.49
2:C:250:MET:O	2:C:253:LEU:HG	2.12	0.49
2:C:444:ARG:NH1	2:C:580:VAL:HG23	2.27	0.49
2:C:44:LEU:HD13	2:C:440:LEU:HD21	1.94	0.49
2:C:480:PRO:O	2:C:485:ILE:HG12	2.11	0.49
2:C:493:VAL:HG12	2:C:494:TYR:CD1	2.47	0.49
5:F:253:MET:CE	5:F:297:MET:HA	2.39	0.49
1:B:47:PRO:HB3	1:B:144:ARG:HD2	1.94	0.49
2:C:361:ILE:N	2:C:361:ILE:HD12	2.27	0.49
2:C:506:PRO:HB2	2:C:572:VAL:HG11	1.92	0.49
2:C:980:LEU:HB3	2:C:995:ALA:HA	1.94	0.49
3:D:76:GLU:H	3:D:76:GLU:CD	2.15	0.49
5:F:462:ARG:HH12	5:F:465:LEU:CD1	2.23	0.49
5:F:465:LEU:HD23	5:F:466:ASP:N	2.26	0.49
2:C:44:LEU:CD1	2:C:440:LEU:HD21	2.42	0.49
2:C:704:MET:HE3	2:C:706:LEU:HD21	1.94	0.49
2:C:895:MET:HG3	2:C:896:PRO:CD	2.39	0.49
3:D:1034:GLU:OE2	3:D:1042:ARG:N	2.44	0.49
3:D:150:THR:O	3:D:154:GLU:HG3	2.13	0.49
3:D:183:GLU:O	3:D:187:GLU:HG2	2.12	0.49
2:C:1029:ASP:OD1	3:D:520:LYS:HD2	2.12	0.49
3:D:651:PHE:C	3:D:653:ASN:H	2.15	0.49
3:D:591:LEU:HD23	3:D:666:THR:HG22	1.94	0.49
3:D:58:TRP:CD1	3:D:68:VAL:HG22	2.47	0.49
3:D:726:SER:OG	3:D:728:VAL:HG23	2.11	0.49
1:A:146:TYR:CG	2:C:734:GLU:HG2	2.47	0.49
1:B:105:VAL:HB	1:B:125:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1103:ILE:HD12	3:D:548:SER:HA	1.93	0.49
2:C:193:VAL:HG12	2:C:205:PHE:HB2	1.94	0.49
3:D:438:LEU:HA	3:D:525:HIS:CD2	2.47	0.49
1:A:130:ASP:OD1	1:A:130:ASP:N	2.44	0.49
1:B:50:ALA:HB3	1:B:168:TYR:HD2	1.77	0.49
2:C:494:TYR:HD2	2:C:572:VAL:HG21	1.76	0.49
2:C:623:LEU:CD1	2:C:623:LEU:H	2.25	0.49
3:D:114:LEU:HG	3:D:312:MET:HE2	1.95	0.49
3:D:373:MET:SD	5:F:256:LEU:HB3	2.53	0.49
8:O:15:DT:H1'	8:O:16:DT:H5''	1.94	0.49
1:A:112:PRO:HB2	1:A:116:VAL:HG23	1.95	0.49
2:C:231:ALA:HB1	2:C:287:LEU:HD11	1.95	0.49
2:C:390:VAL:O	2:C:394:ARG:HB2	2.13	0.49
3:D:28:VAL:HG21	3:D:46:LEU:HD23	1.94	0.49
3:D:527:LEU:HD21	3:D:581:MET:HE3	1.95	0.49
3:D:527:LEU:HD13	3:D:712:VAL:HG12	1.94	0.49
2:C:1012:TYR:CG	3:D:727:GLY:HA3	2.48	0.49
3:D:752:ALA:HB1	3:D:773:LEU:CD2	2.42	0.49
5:F:345:PRO:HA	5:F:348:VAL:CG1	2.42	0.49
5:F:365:ILE:HD12	5:F:366:GLY:N	2.27	0.49
7:J:50:ILE:CG2	7:J:64:LEU:HD11	2.43	0.49
9:P:23:DA:H2''	9:P:24:DA:O4'	2.12	0.49
2:C:882:ASN:HD21	2:C:1019:MET:CE	2.26	0.49
2:C:1043:ILE:HG23	2:C:1044:THR:N	2.28	0.49
2:C:227:VAL:CG2	2:C:268:ILE:HD11	2.42	0.49
2:C:51:SER:HB2	2:C:371:THR:OG1	2.12	0.49
2:C:41:VAL:HG13	2:C:493:VAL:CG1	2.43	0.49
2:C:560:GLU:HG3	2:C:561:PHE:N	2.27	0.49
2:C:758:GLU:CG	2:C:798:THR:HG22	2.34	0.49
2:C:967:VAL:HG23	2:C:968:PHE:H	1.78	0.49
2:C:1032:ILE:HG21	3:D:520:LYS:HD3	1.93	0.49
5:F:215:GLN:O	5:F:219:MET:HG2	2.13	0.49
5:F:324:LEU:CD2	5:F:328:LEU:HD22	2.42	0.49
5:F:462:ARG:HD3	5:F:462:ARG:O	2.13	0.49
1:A:24:GLU:CD	1:A:191:LYS:HD3	2.33	0.49
2:C:454:LEU:HD22	2:C:459:ALA:HB2	1.93	0.49
2:C:876:LEU:HD13	2:C:886:ILE:HG13	1.94	0.49
5:F:423:GLN:HG3	5:F:425:ARG:HE	1.78	0.49
1:A:192:LEU:HD12	1:A:192:LEU:C	2.33	0.49
2:C:32:PHE:O	2:C:34:LYS:HD2	2.13	0.49
2:C:496:ARG:HH21	2:C:521:TYR:HB2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:789:ASP:HA	2:C:830:VAL:CG1	2.43	0.49
2:C:1073:ALA:HB1	3:D:1258:LEU:HG	1.94	0.49
3:D:397:ARG:HG3	3:D:397:ARG:O	2.11	0.49
3:D:88:ARG:O	3:D:322:PRO:HD2	2.12	0.49
5:F:164:ASP:OD1	5:F:166:VAL:N	2.43	0.49
1:A:24:GLU:HB3	1:A:191:LYS:HG3	1.95	0.48
1:B:71:GLU:HB3	1:B:76:ILE:HG13	1.95	0.48
2:C:23:VAL:HB	2:C:26:ALA:HB2	1.94	0.48
2:C:763:ASP:CB	2:C:821:ARG:HH22	2.18	0.48
3:D:236:VAL:HG12	3:D:236:VAL:O	2.13	0.48
7:J:40:PHE:CZ	7:J:58:ASN:HB2	2.47	0.48
3:D:24:SER:O	7:J:57:ARG:HD2	2.13	0.48
2:C:589:GLU:HB3	2:C:968:PHE:CD1	2.48	0.48
3:D:103:HIS:ND1	3:D:105:TRP:HB2	2.28	0.48
3:D:1266:SER:HA	3:D:1269:ARG:NH1	2.26	0.48
3:D:173:ARG:NH2	3:D:201:GLY:HA2	2.29	0.48
3:D:499:ASN:HB2	3:D:509:ILE:HG12	1.95	0.48
1:A:113:PRO:O	1:A:116:VAL:HG22	2.13	0.48
2:C:445:ARG:C	2:C:446:LEU:HD23	2.33	0.48
3:D:116:TYR:CB	3:D:298:VAL:HG11	2.43	0.48
2:C:1064:CYS:O	2:C:1068:GLN:HG3	2.13	0.48
3:D:153:ALA:O	3:D:157:VAL:HG23	2.13	0.48
2:C:1112:PHE:CE2	3:D:1255:ILE:HG22	2.49	0.48
2:C:916:ARG:NH2	10:C:1201:SO4:O1	2.46	0.48
2:C:334:GLU:O	2:C:338:ARG:HG2	2.13	0.48
3:D:1140:GLN:NE2	3:D:1155:ILE:HD12	2.29	0.48
5:F:290:ARG:NH1	11:F:506:EDO:H11	2.29	0.48
1:A:111:VAL:O	1:A:111:VAL:HG23	2.14	0.48
1:A:70:LYS:HB3	1:A:71:GLU:OE1	2.13	0.48
2:C:1034:ALA:O	2:C:1054:PHE:HE2	1.96	0.48
2:C:148:PHE:CE1	2:C:380:ILE:HD11	2.48	0.48
2:C:178:PHE:O	2:C:358:VAL:HG13	2.13	0.48
2:C:792:ILE:HD12	2:C:792:ILE:N	2.29	0.48
3:D:1054:VAL:CG2	3:D:1065:ILE:HG23	2.44	0.48
3:D:590:THR:CG2	3:D:630:ARG:HE	2.25	0.48
3:D:675:LEU:HD21	3:D:718:ALA:CB	2.43	0.48
3:D:884:ILE:HD11	3:D:886:ARG:NE	2.29	0.48
1:A:2:LEU:HD12	1:B:143:GLY:CA	2.42	0.48
1:B:55:ARG:HG2	1:B:137:GLU:HB3	1.96	0.48
2:C:412:ARG:CZ	5:F:322:ARG:HH11	2.27	0.48
2:C:727:ILE:HA	2:C:888:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1193:ARG:O	3:D:1195:VAL:N	2.47	0.48
3:D:222:ILE:HG23	3:D:244:LEU:HD23	1.95	0.48
5:F:179:LEU:HB3	5:F:183:GLU:HB2	1.95	0.48
1:B:213:GLY:HA2	1:B:216:VAL:HG12	1.96	0.48
2:C:1045:GLN:HG3	2:C:1090:ARG:HH21	1.79	0.48
2:C:203:LEU:HD11	2:C:217:ILE:HB	1.96	0.48
3:D:461:VAL:HG23	3:D:472:ALA:HB2	1.96	0.48
1:A:68:GLY:HA3	1:A:129:ASN:HD21	1.79	0.48
1:A:55:ARG:HH22	1:A:158:GLU:HB2	1.79	0.48
1:B:112:PRO:CB	1:B:116:VAL:HG23	2.43	0.48
2:C:176:VAL:HG12	2:C:195:VAL:CG2	2.30	0.48
2:C:41:VAL:HG13	2:C:493:VAL:HG12	1.96	0.48
2:C:29:ARG:HD3	2:C:964:ALA:HB2	1.95	0.48
3:D:735:VAL:CG2	3:D:798:ILE:HD11	2.44	0.48
3:D:706:ILE:HD11	4:E:36:PRO:HA	1.94	0.48
1:A:64:THR:O	1:A:73:VAL:HG23	2.14	0.48
3:D:28:VAL:CG1	3:D:319:VAL:HG21	2.44	0.48
5:F:199:GLN:HG2	7:J:82:TRP:CE2	2.49	0.48
5:F:324:LEU:HB3	5:F:332:PRO:HG3	1.96	0.48
8:O:6:DA:C1'	8:O:7:DC:H5'	2.44	0.48
1:A:84:VAL:HG12	1:A:120:ASN:CG	2.35	0.47
2:C:1039:PRO:HB2	2:C:1048:LEU:HD21	1.96	0.47
2:C:571:ASP:HB3	2:C:576:GLN:HE21	1.78	0.47
2:C:472:GLY:H	2:C:577:MET:HA	1.78	0.47
2:C:609:LEU:HD12	2:C:708:LYS:HE3	1.94	0.47
2:C:602:MET:CE	2:C:883:LYS:HB3	2.33	0.47
3:D:1181:LEU:HD22	3:D:1207:VAL:HG11	1.96	0.47
5:F:277:LYS:HB3	5:F:279:TYR:CD2	2.49	0.47
1:B:32:TYR:CE1	2:C:1005:ARG:HD3	2.49	0.47
1:B:89:ASP:O	1:B:90:ASP:HB2	2.14	0.47
2:C:421:PHE:O	2:C:425:SER:HB3	2.14	0.47
1:A:100:GLN:OE1	1:A:101:GLY:N	2.35	0.47
2:C:1045:GLN:HG2	2:C:1087:THR:CG2	2.35	0.47
2:C:531:VAL:HG22	2:C:552:VAL:CG1	2.43	0.47
2:C:774:ASP:HA	2:C:782:ARG:NH2	2.29	0.47
1:A:40:ARG:NH2	2:C:894:ASP:HB3	2.29	0.47
2:C:31:SER:HA	2:C:964:ALA:O	2.14	0.47
7:J:74:LYS:HB2	7:J:74:LYS:HE2	1.73	0.47
1:A:93:VAL:HG22	1:A:113:PRO:HG2	1.96	0.47
1:B:147:VAL:O	1:B:147:VAL:HG13	2.15	0.47
2:C:531:VAL:HG13	2:C:552:VAL:CG1	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:118:LEU:CB	3:D:120:LEU:HD13	2.44	0.47
3:D:133:ALA:CB	3:D:234:LEU:HD21	2.45	0.47
3:D:92:MET:HG2	3:D:321:PRO:HD3	1.97	0.47
3:D:945:ASP:N	3:D:946:PRO:HD2	2.29	0.47
3:D:1275:PRO:CG	4:E:76:VAL:HG11	2.42	0.47
5:F:306:ILE:HG22	5:F:310:MET:HB3	1.97	0.47
9:P:20:DG:H2''	9:P:21:DT:H5'	1.96	0.47
1:A:83:LEU:HD23	1:A:123:MET:SD	2.54	0.47
1:B:21:PHE:HB2	1:B:194:ILE:CG2	2.44	0.47
2:C:154:LYS:HD2	2:C:630:GLY:HA3	1.95	0.47
2:C:935:TRP:CA	2:C:983:THR:HG23	2.44	0.47
3:D:102:THR:HG23	3:D:258:ALA:HB2	1.96	0.47
3:D:1252:ASN:HB3	3:D:1257:LYS:HB3	1.97	0.47
3:D:104:ILE:HD11	3:D:386:ARG:HG2	1.96	0.47
3:D:327:MET:CE	5:F:304:ILE:HD11	2.42	0.47
2:C:126:VAL:HG12	2:C:127:THR:N	2.30	0.47
2:C:159:ILE:HG13	2:C:422:PHE:HB3	1.96	0.47
3:D:753:ASP:O	3:D:757:ARG:N	2.42	0.47
3:D:915:VAL:O	3:D:920:PHE:HD2	1.98	0.47
2:C:433:GLN:HE21	2:C:670:ASN:N	2.10	0.47
2:C:587:PHE:HB3	2:C:590:HIS:HD2	1.80	0.47
3:D:278:ARG:HA	3:D:281:ILE:HD11	1.97	0.47
2:C:973:GLU:CB	3:D:732:MET:HE3	2.45	0.47
2:C:1043:ILE:HD13	3:D:412:ARG:HH22	1.79	0.47
2:C:36:ARG:O	2:C:38:PRO:HD3	2.15	0.47
2:C:70:GLU:CD	2:C:70:GLU:H	2.17	0.47
5:F:325:LEU:HD23	5:F:325:LEU:O	2.15	0.47
1:B:139:VAL:HG21	1:B:161:ARG:HH21	1.80	0.47
2:C:510:VAL:CG1	2:C:567:VAL:HG12	2.44	0.47
2:C:530:HIS:HB3	2:C:568:ASP:OD2	2.15	0.47
2:C:792:ILE:HD12	2:C:792:ILE:H	1.79	0.47
2:C:780:ILE:HD13	2:C:841:ILE:HG21	1.97	0.47
3:D:39:LEU:HD13	3:D:335:PHE:HZ	1.80	0.47
3:D:613:SER:N	3:D:617:GLU:OE1	2.43	0.47
3:D:686:GLN:HG3	3:D:686:GLN:O	2.15	0.47
3:D:735:VAL:HG11	3:D:816:LEU:CD2	2.45	0.47
5:F:214:GLN:HE21	5:F:214:GLN:HA	1.80	0.47
3:D:79:GLY:HA2	7:J:54:TRP:CH2	2.50	0.47
3:D:25:TYR:C	7:J:57:ARG:HG3	2.34	0.47
1:B:182:ARG:O	1:B:186:ARG:O	2.33	0.47
2:C:709:ASN:C	2:C:710:LEU:HD12	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:723:GLU:O	2:C:724:ASP:HB2	2.15	0.47
2:C:805:LEU:HD22	2:C:805:LEU:N	2.30	0.47
1:A:147:VAL:HG13	1:A:147:VAL:O	2.15	0.47
2:C:552:VAL:HG12	2:C:553:ARG:N	2.30	0.47
2:C:566:GLN:OE1	2:C:566:GLN:HA	2.15	0.47
2:C:710:LEU:HD13	2:C:1021:ILE:CG1	2.45	0.47
3:D:1063:PHE:HB2	3:D:1081:LEU:HB2	1.97	0.47
3:D:12:ILE:HG12	3:D:1221:TRP:CZ2	2.50	0.47
3:D:143:MET:HG2	3:D:251:TYR:CE1	2.50	0.47
3:D:245:GLN:O	3:D:249:GLY:HA3	2.15	0.47
3:D:330:LEU:HD22	3:D:330:LEU:N	2.29	0.47
3:D:406:LEU:HB3	3:D:413:PHE:HE1	1.79	0.47
3:D:694:ARG:CZ	3:D:694:ARG:HB3	2.44	0.47
5:F:291:GLN:HG3	5:F:292:ALA:N	2.30	0.47
8:O:19:DA:H2'	8:O:20:DT:C6	2.50	0.47
1:A:106:THR:HA	1:A:125:ILE:HD13	1.98	0.46
1:B:73:VAL:O	1:B:77:ILE:HG13	2.15	0.46
3:D:48:CYS:SG	3:D:50:LYS:HB3	2.55	0.46
3:D:612:TYR:OH	3:D:627:LEU:HG	2.15	0.46
1:A:113:PRO:HD2	1:A:116:VAL:CG2	2.43	0.46
1:A:70:LYS:CB	1:A:127:THR:HG23	2.39	0.46
1:B:102:PRO:CG	1:B:131:LYS:H	2.27	0.46
2:C:141:GLN:CD	2:C:406:GLN:HG2	2.35	0.46
2:C:434:ASN:O	2:C:608:PRO:HD3	2.15	0.46
3:D:231:PRO:O	3:D:232:LYS:HB2	2.15	0.46
3:D:646:LEU:HD23	3:D:646:LEU:O	2.15	0.46
3:D:58:TRP:CZ3	3:D:71:LYS:HE3	2.50	0.46
7:J:40:PHE:HZ	7:J:58:ASN:HB2	1.80	0.46
8:O:4:DT:H2''	8:O:5:DG:C8	2.49	0.46
1:A:192:LEU:HD12	1:A:192:LEU:O	2.15	0.46
1:B:137:GLU:C	1:B:138:LEU:HD12	2.36	0.46
1:B:74:THR:OG1	3:D:608:GLU:HG3	2.15	0.46
3:D:886:ARG:HH12	14:D:2012:GLU:CB	2.28	0.46
5:F:449:MET:O	5:F:453:ARG:HG3	2.15	0.46
1:A:43:LEU:HD11	1:A:174:VAL:HB	1.96	0.46
1:A:56:ILE:HB	1:A:59:VAL:CG2	2.45	0.46
2:C:1044:THR:OG1	2:C:1046:GLN:HG3	2.16	0.46
12:C:1205:RFP:H323	12:C:1205:RFP:H20C	1.71	0.46
2:C:176:VAL:O	2:C:176:VAL:HG23	2.14	0.46
2:C:777:GLU:CD	2:C:777:GLU:H	2.18	0.46
2:C:727:ILE:HG22	2:C:888:LYS:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:30:VAL:CG1	2:C:954:LEU:HG	2.44	0.46
5:F:404:THR:HB	5:F:457:ARG:HH21	1.80	0.46
7:J:69:VAL:N	7:J:70:PRO:HD3	2.30	0.46
2:C:491:LEU:HG	2:C:495:ALA:HB3	1.98	0.46
2:C:891:PRO:HB2	2:C:893:GLU:CG	2.44	0.46
3:D:1231:THR:O	3:D:1235:THR:HG23	2.15	0.46
3:D:12:ILE:HD12	3:D:1237:ALA:CB	2.46	0.46
3:D:287:GLN:HG3	3:D:288:LYS:HD3	1.97	0.46
5:F:409:GLU:O	5:F:413:VAL:HG23	2.16	0.46
1:B:226:ASN:O	1:B:227:ALA:HB3	2.15	0.46
1:B:32:TYR:CZ	2:C:1005:ARG:HD3	2.51	0.46
2:C:404:THR:H	2:C:407:THR:HG1	1.60	0.46
2:C:614:ALA:HA	2:C:705:ALA:CB	2.45	0.46
3:D:131:PHE:C	3:D:256:MET:HE1	2.35	0.46
3:D:262:LYS:HG3	3:D:310:MET:CE	2.46	0.46
5:F:445:GLU:O	5:F:449:MET:HG2	2.15	0.46
1:B:52:THR:HG21	1:B:141:GLU:OE2	2.15	0.46
2:C:1035:ARG:NH2	2:C:1047:PRO:HB3	2.30	0.46
2:C:204:GLU:HB2	2:C:216:ARG:NH1	2.30	0.46
2:C:143:VAL:HA	2:C:406:GLN:HE22	1.81	0.46
3:D:171:GLU:O	3:D:175:GLN:HG3	2.16	0.46
3:D:819:MET:CE	3:D:821:GLY:HA2	2.46	0.46
1:A:45:SER:O	1:A:47:PRO:HD3	2.16	0.46
1:B:210:SER:O	1:B:214:THR:HG23	2.16	0.46
1:B:28:PRO:HA	1:B:29:GLY:HA2	1.51	0.46
2:C:375:LEU:CD1	2:C:427:LEU:HD22	2.44	0.46
3:D:1031:ARG:CZ	3:D:1035:LEU:HD21	2.46	0.46
3:D:108:LYS:HG3	3:D:108:LYS:O	2.16	0.46
3:D:1275:PRO:CB	4:E:79:LEU:HD11	2.43	0.46
7:J:73:LYS:C	7:J:74:LYS:HG3	2.36	0.46
1:B:77:ILE:O	1:B:81:LYS:HG3	2.16	0.46
2:C:935:TRP:HA	2:C:983:THR:H	1.81	0.46
3:D:23:TRP:HB3	3:D:92:MET:HE3	1.98	0.46
2:C:1047:PRO:HD2	3:D:421:ARG:O	2.15	0.46
3:D:452:PHE:CE1	3:D:491:ILE:HG12	2.51	0.46
3:D:735:VAL:HG12	3:D:840:ARG:CD	2.42	0.46
3:D:920:PHE:CZ	3:D:948:ILE:HG13	2.51	0.46
4:E:55:ALA:O	4:E:59:ARG:HG2	2.16	0.46
5:F:440:ARG:O	5:F:444:ILE:HG13	2.15	0.46
1:A:9:LEU:HD13	1:A:23:ILE:HG12	1.97	0.46
2:C:445:ARG:NH1	12:C:1205:RFP:C30	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:712:VAL:HA	2:C:906:ILE:HG13	1.98	0.46
3:D:320:ILE:CG1	3:D:321:PRO:HD2	2.45	0.46
3:D:581:MET:HE2	3:D:716:LYS:CA	2.34	0.46
5:F:345:PRO:HA	5:F:348:VAL:HG13	1.98	0.46
5:F:348:VAL:O	5:F:352:GLN:HG3	2.16	0.46
1:A:92:PRO:HB3	1:A:141:GLU:HG3	1.98	0.45
1:A:174:VAL:O	2:C:901:GLY:HA3	2.16	0.45
2:C:336:LEU:HD23	2:C:336:LEU:O	2.16	0.45
2:C:343:GLN:NE2	2:C:345:SER:O	2.49	0.45
2:C:627:ILE:HD12	2:C:628:ASP:N	2.31	0.45
2:C:1074:TYR:CZ	3:D:1258:LEU:HD21	2.51	0.45
3:D:1249:LEU:HA	3:D:1260:PRO:HD2	1.98	0.45
3:D:190:LYS:HD2	3:D:192:ASP:HB3	1.97	0.45
3:D:238:GLU:HA	3:D:241:TYR:HB3	1.97	0.45
1:A:107:ALA:HB3	1:A:121:PRO:HA	1.99	0.45
2:C:166:VAL:HG11	2:C:372:VAL:HG23	1.99	0.45
2:C:473:ARG:NH1	2:C:524:ALA:HA	2.31	0.45
2:C:523:THR:HG23	2:C:526:GLU:OE2	2.15	0.45
3:D:1001:SER:O	3:D:1150:ILE:HD12	2.17	0.45
3:D:191:SER:O	3:D:195:ARG:HG2	2.16	0.45
3:D:278:ARG:O	3:D:281:ILE:HD12	2.16	0.45
8:O:14:DG:H3'	1:T:258:VAL:CG1	2.45	0.45
1:A:137:GLU:C	1:A:138:LEU:HD12	2.37	0.45
1:A:9:LEU:HD13	1:A:23:ILE:HG13	1.97	0.45
2:C:32:PHE:HE1	2:C:963:VAL:CG1	2.29	0.45
3:D:1010:THR:OG1	3:D:1010:THR:O	2.30	0.45
3:D:630:ARG:HD3	11:D:2011:EDO:H21	1.98	0.45
3:D:796:ASN:HD22	3:D:799:ILE:H	1.64	0.45
3:D:875:ARG:HH22	3:D:1033:GLN:CD	2.20	0.45
1:A:56:ILE:HG12	1:A:136:VAL:CB	2.42	0.45
1:B:185:GLN:HE21	1:B:185:GLN:HB2	1.53	0.45
2:C:444:ARG:NH1	2:C:580:VAL:CG2	2.79	0.45
2:C:481:GLU:OE2	2:C:598:MET:HG2	2.17	0.45
3:D:95:ILE:HD13	3:D:348:ILE:HG12	1.98	0.45
3:D:656:LYS:HB2	3:D:659:ASP:CB	2.46	0.45
3:D:664:GLU:O	3:D:664:GLU:HG3	2.17	0.45
4:E:80:VAL:HG12	4:E:81:GLU:N	2.32	0.45
7:J:69:VAL:O	7:J:69:VAL:HG12	2.15	0.45
1:B:96:TYR:O	1:B:110:ILE:HG13	2.16	0.45
1:B:230:GLU:OE1	1:B:230:GLU:HA	2.17	0.45
2:C:203:LEU:C	2:C:204:GLU:HG3	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:554:LYS:O	2:C:557:GLY:HA2	2.15	0.45
2:C:623:LEU:HD13	2:C:624:ARG:H	1.81	0.45
3:D:1170:ASP:O	3:D:1202:ALA:HA	2.16	0.45
4:E:26:TYR:HE1	4:E:29:PRO:HD3	1.80	0.45
1:A:111:VAL:CG2	1:A:111:VAL:O	2.65	0.45
1:A:46:ILE:HD12	1:A:210:SER:OG	2.17	0.45
1:B:174:VAL:HA	1:B:195:ASP:O	2.16	0.45
2:C:481:GLU:HG2	2:C:597:LEU:HD21	1.98	0.45
1:T:264:LEU:O	1:T:269:VAL:HG22	2.15	0.45
2:C:984:LEU:CD1	2:C:991:VAL:HG23	2.36	0.45
3:D:1181:LEU:HD11	3:D:1213:LYS:HE2	1.99	0.45
3:D:1219:ASP:O	3:D:1242:ARG:NH2	2.50	0.45
2:C:1043:ILE:HD13	3:D:412:ARG:NH2	2.32	0.45
2:C:1103:ILE:CD1	3:D:547:LEU:HB3	2.46	0.45
3:D:796:ASN:ND2	3:D:798:ILE:HB	2.25	0.45
3:D:706:ILE:CD1	4:E:36:PRO:HB3	2.42	0.45
1:A:24:GLU:HB3	1:A:191:LYS:CG	2.46	0.45
1:B:22:VAL:CG1	1:B:193:ILE:HD12	2.46	0.45
2:C:898:LEU:HD23	2:C:1001:LEU:HD23	1.99	0.45
2:C:1117:LYS:HD2	2:C:1117:LYS:HA	1.72	0.45
2:C:158:ILE:HD12	2:C:158:ILE:N	2.31	0.45
3:D:288:LYS:HD2	3:D:291:ARG:NH2	2.11	0.45
7:J:28:GLN:CG	7:J:46:ASP:HA	2.47	0.45
1:T:251:ILE:HA	1:T:272:VAL:CG2	2.40	0.45
1:B:8:THR:O	1:B:23:ILE:HA	2.17	0.45
2:C:51:SER:OG	2:C:371:THR:HG23	2.17	0.45
2:C:947:ALA:O	2:C:951:PRO:HD2	2.17	0.45
3:D:321:PRO:HD2	3:D:324:LEU:HD12	1.97	0.45
5:F:187:LEU:O	5:F:191:ILE:HG13	2.17	0.45
1:A:152:ASN:HD21	2:C:837:LYS:NZ	2.14	0.45
1:A:54:ILE:C	1:A:54:ILE:HD12	2.37	0.45
2:C:432:ASP:HA	2:C:671:HIS:NE2	2.32	0.45
2:C:44:LEU:H	2:C:44:LEU:HG	1.56	0.45
2:C:714:ILE:HD13	2:C:922:ILE:CD1	2.47	0.45
2:C:85:SER:HA	2:C:86:PRO:HA	1.70	0.45
2:C:984:LEU:O	2:C:984:LEU:HG	2.17	0.45
3:D:276:SER:O	3:D:280:VAL:HG23	2.17	0.45
2:C:723:GLU:HB3	3:D:536:PHE:HD1	1.82	0.45
3:D:704:PRO:HB3	4:E:38:ASP:CG	2.37	0.45
8:O:16:DT:O2	9:P:11:DA:H2	2.00	0.45
2:C:1126:VAL:O	2:C:1126:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:608:PRO:HA	2:C:698:CYS:SG	2.56	0.44
3:D:1123:LEU:HD22	3:D:1208:LEU:HB2	1.98	0.44
3:D:190:LYS:CE	3:D:192:ASP:HB3	2.47	0.44
3:D:972:GLY:HA2	10:D:2004:SO4:O2	2.17	0.44
3:D:505:HIS:ND1	3:D:507:LEU:HB2	2.32	0.44
3:D:525:HIS:O	3:D:528:VAL:HG22	2.17	0.44
3:D:770:ASN:O	3:D:774:VAL:HG23	2.17	0.44
5:F:365:ILE:HG23	5:F:365:ILE:O	2.16	0.44
2:C:229:LEU:HD12	2:C:229:LEU:O	2.16	0.44
2:C:591:ASP:OD2	2:C:880:HIS:ND1	2.41	0.44
2:C:712:VAL:HG11	2:C:925:THR:HG23	1.99	0.44
3:D:1056:LEU:HD23	3:D:1057:GLU:N	2.31	0.44
3:D:1132:GLN:NE2	3:D:1163:LEU:HD12	2.32	0.44
3:D:357:LEU:HD13	3:D:366:ILE:HG22	1.98	0.44
3:D:436:LEU:O	3:D:716:LYS:NZ	2.51	0.44
1:B:111:VAL:O	1:B:111:VAL:HG13	2.17	0.44
1:B:47:PRO:HA	1:B:144:ARG:CG	2.42	0.44
2:C:1045:GLN:CG	2:C:1090:ARG:HH21	2.30	0.44
2:C:634:VAL:HG13	2:C:691:GLN:O	2.18	0.44
3:D:1056:LEU:HD21	3:D:1063:PHE:CE1	2.52	0.44
3:D:759:TYR:CD2	3:D:769:ARG:HD3	2.52	0.44
1:B:74:THR:O	1:B:78:LEU:HG	2.17	0.44
2:C:323:THR:OG1	2:C:324:LEU:N	2.50	0.44
2:C:448:ALA:O	2:C:454:LEU:HD12	2.17	0.44
2:C:498:ASN:ND2	2:C:500:PHE:HB2	2.32	0.44
2:C:534:GLN:HE21	2:C:534:GLN:CA	2.21	0.44
3:D:1056:LEU:HD23	3:D:1057:GLU:H	1.81	0.44
3:D:1086:ARG:H	3:D:1086:ARG:CD	2.11	0.44
5:F:373:LEU:O	5:F:373:LEU:HD23	2.18	0.44
1:T:269:VAL:HG23	1:T:269:VAL:O	2.17	0.44
1:A:49:ALA:HB2	1:A:87:SER:H	1.83	0.44
2:C:344:THR:HG22	2:C:344:THR:O	2.18	0.44
2:C:505:THR:CG2	2:C:506:PRO:HD2	2.47	0.44
2:C:772:LEU:N	2:C:772:LEU:HD12	2.33	0.44
3:D:825:ASN:CB	3:D:826:PRO:HD2	2.48	0.44
5:F:271:GLU:HA	7:J:81:HIS:NE2	2.33	0.44
5:F:373:LEU:HD23	5:F:373:LEU:C	2.38	0.44
1:A:172:LEU:C	1:A:172:LEU:HD23	2.38	0.44
2:C:1014:VAL:HG13	3:D:729:THR:CG2	2.47	0.44
2:C:572:VAL:HG22	2:C:576:GLN:CD	2.38	0.44
2:C:986:ASN:OD1	2:C:986:ASN:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1069:ALA:HB3	3:D:506:ARG:HB3	1.99	0.44
3:D:988:VAL:CG2	3:D:992:GLU:HG3	2.46	0.44
9:P:4:DA:H2"	9:P:5:DC:H6	1.82	0.44
1:A:50:ALA:HB3	1:A:168:TYR:CE1	2.52	0.44
2:C:1066:ALA:HB1	3:D:506:ARG:HA	1.99	0.44
2:C:1070:TYR:CD1	3:D:559:MET:HG2	2.52	0.44
3:D:1132:GLN:CG	3:D:1163:LEU:HD12	2.47	0.44
3:D:929:VAL:O	3:D:929:VAL:HG23	2.18	0.44
5:F:231:ASN:O	5:F:235:GLU:HG3	2.18	0.44
8:O:6:DA:H2"	8:O:7:DC:OP2	2.17	0.44
2:C:119:THR:HB	2:C:160:ASN:H	1.83	0.44
2:C:680:ILE:HG12	2:C:693:ILE:O	2.18	0.44
3:D:110:VAL:HG13	3:D:110:VAL:O	2.18	0.44
3:D:1165:ARG:HE	3:D:1209:MET:HE1	1.83	0.44
3:D:1272:GLN:OE1	3:D:1272:GLN:HA	2.18	0.44
3:D:556:ARG:O	3:D:560:LEU:HB2	2.17	0.44
3:D:744:ILE:O	3:D:748:HIS:HD2	2.01	0.44
5:F:199:GLN:HG2	7:J:82:TRP:CZ2	2.53	0.44
2:C:1036:SER:HB3	3:D:450:GLU:O	2.17	0.44
3:D:143:MET:CE	3:D:251:TYR:HA	2.48	0.44
3:D:573:PRO:HG2	3:D:576:MET:HE2	1.99	0.44
2:C:1011:PRO:HB2	2:C:1012:TYR:HD2	1.82	0.43
2:C:614:ALA:H	2:C:700:GLN:NE2	2.16	0.43
2:C:641:ILE:CG2	2:C:644:VAL:HG13	2.48	0.43
2:C:846:ARG:N	2:C:857:ASN:O	2.50	0.43
3:D:1057:GLU:HB2	3:D:1064:LYS:HB3	1.99	0.43
3:D:397:ARG:NH2	5:F:360:SER:OG	2.50	0.43
3:D:638:THR:HG22	3:D:660:ALA:HB2	2.00	0.43
7:J:98:LEU:HG	7:J:102:LEU:CD1	2.47	0.43
2:C:1057:GLN:O	3:D:421:ARG:HA	2.17	0.43
2:C:508:ARG:HD2	2:C:570:MET:HE3	1.99	0.43
3:D:444:PRO:HD2	3:D:447:MET:HE2	2.00	0.43
1:A:215:LEU:HA	1:A:215:LEU:HD12	1.84	0.43
1:B:24:GLU:HA	1:B:25:PRO:HA	1.67	0.43
2:C:335:TYR:HD1	2:C:335:TYR:O	2.00	0.43
2:C:94:MET:SD	2:C:395:MET:HB3	2.57	0.43
2:C:767:VAL:HG21	2:C:772:LEU:HD11	1.99	0.43
2:C:780:ILE:HG13	2:C:780:ILE:O	2.17	0.43
3:D:115:GLY:O	3:D:119:ASP:N	2.52	0.43
3:D:12:ILE:HD12	3:D:1237:ALA:HB1	2.00	0.43
3:D:65:TYR:HB3	3:D:70:PHE:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:65:ILE:HG22	7:J:65:ILE:O	2.18	0.43
1:A:54:ILE:CD1	1:A:162:ILE:HB	2.48	0.43
1:A:219:PHE:CE1	1:B:38:LEU:HD21	2.52	0.43
5:F:310:MET:O	5:F:313:VAL:HG13	2.17	0.43
7:J:88:ARG:HG3	7:J:89:ARG:N	2.33	0.43
1:A:72:ASP:OD1	1:A:75:ASP:N	2.41	0.43
1:B:138:LEU:N	1:B:138:LEU:HD12	2.33	0.43
1:B:34:LEU:O	1:B:38:LEU:HD23	2.19	0.43
1:B:55:ARG:O	1:B:55:ARG:HG3	2.18	0.43
2:C:100:ASP:OD2	2:C:102:ARG:NH2	2.50	0.43
2:C:169:GLN:HB2	2:C:427:LEU:CD2	2.48	0.43
2:C:614:ALA:HA	2:C:705:ALA:HB2	2.00	0.43
2:C:973:GLU:HA	3:D:732:MET:HE3	2.00	0.43
3:D:1005:PRO:HG3	3:D:1150:ILE:HD11	2.00	0.43
3:D:527:LEU:HD11	3:D:712:VAL:HG12	2.00	0.43
3:D:85:ALA:O	3:D:88:ARG:HB2	2.18	0.43
3:D:937:ILE:HD12	3:D:951:LEU:CG	2.42	0.43
3:D:948:ILE:O	3:D:952:LEU:HD22	2.19	0.43
5:F:295:ARG:NH2	8:O:24:DG:O6	2.51	0.43
1:B:50:ALA:HB3	1:B:168:TYR:CD2	2.54	0.43
2:C:1048:LEU:CD2	2:C:1048:LEU:H	2.19	0.43
2:C:126:VAL:HG12	2:C:127:THR:H	1.82	0.43
2:C:498:ASN:HD22	2:C:500:PHE:HB2	1.82	0.43
2:C:475:CYS:HB2	2:C:579:SER:HB3	1.99	0.43
2:C:780:ILE:HD11	2:C:841:ILE:HD13	2.00	0.43
2:C:720:HIS:CE1	2:C:888:LYS:HD3	2.53	0.43
3:D:589:THR:OG1	3:D:686:GLN:HA	2.18	0.43
3:D:778:GLN:HE21	3:D:778:GLN:HA	1.83	0.43
7:J:28:GLN:N	7:J:44:PHE:O	2.50	0.43
5:F:196:TYR:HA	7:J:82:TRP:CZ3	2.53	0.43
1:A:106:THR:C	1:A:125:ILE:HD13	2.39	0.43
2:C:291:PHE:HB3	2:C:324:LEU:CD1	2.48	0.43
2:C:644:VAL:O	2:C:644:VAL:HG23	2.18	0.43
2:C:780:ILE:HD12	2:C:781:VAL:O	2.19	0.43
2:C:797:VAL:HG11	2:C:823:VAL:CG2	2.49	0.43
2:C:945:ASP:N	2:C:945:ASP:OD1	2.50	0.43
3:D:886:ARG:HH12	14:D:2012:GLU:HB3	1.83	0.43
3:D:243:GLU:O	3:D:247:ARG:HG3	2.19	0.43
1:A:8:THR:OG1	1:A:24:GLU:O	2.29	0.43
1:A:84:VAL:HG13	1:A:84:VAL:O	2.19	0.43
1:B:196:VAL:HG13	1:B:196:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1078:GLU:HG3	2:C:1082:ILE:HD11	2.00	0.43
2:C:178:PHE:CD1	2:C:193:VAL:HB	2.54	0.43
2:C:376:ILE:HD13	2:C:421:PHE:CE2	2.53	0.43
2:C:534:GLN:HB2	2:C:551:MET:HB2	2.01	0.43
2:C:959:ALA:O	2:C:960:ASP:HB2	2.18	0.43
5:F:176:VAL:HG12	5:F:177:ALA:N	2.33	0.43
8:O:12:DG:H1'	8:O:13:DT:H5''	2.01	0.43
2:C:65:ALA:HB1	2:C:70:GLU:OE1	2.19	0.43
3:D:1081:LEU:HB3	3:D:1113:MET:SD	2.59	0.43
3:D:716:LYS:HE3	3:D:717:ASP:OD1	2.18	0.43
2:C:275:GLY:O	5:F:171:LYS:HD2	2.18	0.43
1:B:97:LEU:HB3	1:B:136:VAL:CG1	2.49	0.43
1:B:38:LEU:O	1:B:42:LEU:HD13	2.18	0.43
12:C:1205:RFP:O12	12:C:1205:RFP:O4	2.35	0.43
2:C:177:TYR:CZ	2:C:366:ASN:HB3	2.53	0.43
2:C:493:VAL:HG23	2:C:578:VAL:O	2.18	0.43
2:C:648:TYR:CE2	2:C:650:THR:HG23	2.53	0.43
2:C:437:LEU:HD12	2:C:706:LEU:HD11	2.01	0.43
3:D:119:ASP:C	3:D:120:LEU:HD12	2.40	0.43
3:D:460:LEU:HD12	3:D:460:LEU:C	2.40	0.43
3:D:650:LEU:HB3	3:D:651:PHE:CD2	2.54	0.43
3:D:875:ARG:HD2	3:D:1212:THR:OG1	2.18	0.43
8:O:2:DC:H2'	8:O:3:DT:C7	2.49	0.43
2:C:1003:ASP:HB2	2:C:1010:PHE:CZ	2.54	0.42
3:D:114:LEU:HG	3:D:312:MET:CE	2.49	0.42
3:D:573:PRO:HG2	3:D:576:MET:HE3	1.99	0.42
3:D:716:LYS:HB3	3:D:716:LYS:HE2	1.81	0.42
3:D:819:MET:HE2	3:D:821:GLY:HA2	2.00	0.42
5:F:349:LEU:HA	5:F:349:LEU:HD12	1.80	0.42
5:F:416:ARG:HA	5:F:430:ILE:HD11	2.01	0.42
1:T:279:THR:HG23	1:T:282:ASP:H	1.83	0.42
2:C:602:MET:CE	2:C:1024:LEU:HD21	2.45	0.42
2:C:217:ILE:HD11	2:C:272:LEU:HD11	2.01	0.42
2:C:299:LEU:HD12	2:C:299:LEU:C	2.39	0.42
2:C:475:CYS:HA	2:C:577:MET:O	2.19	0.42
2:C:648:TYR:CD2	2:C:650:THR:HG23	2.54	0.42
2:C:748:ILE:HD11	2:C:796:LYS:HZ3	1.82	0.42
2:C:895:MET:HB2	2:C:895:MET:HE2	1.68	0.42
3:D:1069:PRO:HB2	3:D:1073:GLY:H	1.83	0.42
3:D:656:LYS:NZ	3:D:656:LYS:O	2.45	0.42
3:D:676:LEU:HD12	3:D:676:LEU:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:106:LYS:CE	7:J:106:LYS:HA	2.22	0.42
1:B:30:PHE:HA	1:B:33:THR:CG2	2.49	0.42
2:C:1048:LEU:HD23	2:C:1048:LEU:N	2.22	0.42
2:C:788:ARG:O	2:C:830:VAL:HG11	2.20	0.42
3:D:1160:ARG:O	3:D:1164:ARG:HG3	2.19	0.42
3:D:203:ARG:NE	3:D:203:ARG:HA	2.32	0.42
3:D:133:ALA:HB3	3:D:234:LEU:HD21	2.01	0.42
3:D:513:GLU:OE1	4:E:32:ILE:HG12	2.19	0.42
3:D:889:ASP:OD2	3:D:962:ARG:NH2	2.52	0.42
4:E:95:GLU:HB3	4:E:101:LEU:CD2	2.49	0.42
1:A:82:GLY:CA	1:A:123:MET:HE1	2.49	0.42
2:C:1012:TYR:HB3	2:C:1013:PRO:HD2	2.01	0.42
2:C:508:ARG:HD2	2:C:570:MET:CE	2.50	0.42
3:D:103:HIS:HB3	3:D:106:TYR:HD2	1.85	0.42
3:D:1161:GLN:HA	3:D:1164:ARG:HD3	2.00	0.42
3:D:302:PHE:CE2	3:D:309:PRO:HA	2.55	0.42
5:F:211:LEU:HB2	5:F:216:ARG:HD2	1.99	0.42
3:D:397:ARG:HH21	5:F:360:SER:CB	2.32	0.42
1:A:57:ASP:N	1:A:57:ASP:OD1	2.52	0.42
1:A:210:SER:HB3	1:B:229:SER:CB	2.48	0.42
1:B:63:PHE:CD1	1:B:63:PHE:N	2.87	0.42
2:C:217:ILE:HG13	2:C:217:ILE:O	2.18	0.42
2:C:494:TYR:HB3	2:C:506:PRO:CG	2.46	0.42
2:C:876:LEU:N	2:C:876:LEU:HD12	2.35	0.42
2:C:900:ASP:OD1	2:C:986:ASN:ND2	2.52	0.42
2:C:88:GLU:CG	2:C:92:GLY:HA2	2.39	0.42
3:D:667:LEU:O	3:D:667:LEU:HD23	2.20	0.42
2:C:41:VAL:HG22	2:C:494:TYR:CE1	2.45	0.42
2:C:510:VAL:HG11	2:C:567:VAL:CG1	2.49	0.42
2:C:991:VAL:HG12	2:C:993:VAL:H	1.84	0.42
3:D:246:ASP:OD1	3:D:246:ASP:N	2.52	0.42
3:D:54:PRO:HG3	3:D:81:GLU:O	2.19	0.42
4:E:98:GLY:O	4:E:100:LEU:HD12	2.19	0.42
5:F:230:LYS:O	5:F:234:LEU:HG	2.20	0.42
8:O:11:DA:H2"	8:O:12:DG:C5'	2.49	0.42
1:A:125:ILE:N	1:A:125:ILE:HD12	2.33	0.42
1:B:213:GLY:HA2	1:B:216:VAL:CG1	2.50	0.42
1:A:40:ARG:HD3	1:B:33:THR:CB	2.49	0.42
2:C:180:GLU:O	2:C:180:GLU:HG3	2.19	0.42
2:C:613:GLU:HB3	2:C:708:LYS:CD	2.50	0.42
2:C:665:LYS:NZ	2:C:677:GLN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:331:ASP:OD1	3:D:331:ASP:N	2.52	0.42
3:D:806:ALA:O	11:D:2007:EDO:O2	2.30	0.42
3:D:813:THR:HG22	3:D:813:THR:O	2.20	0.42
5:F:426:THR:OG1	5:F:429:GLU:HG3	2.20	0.42
1:B:107:ALA:HB3	1:B:121:PRO:HA	2.01	0.42
1:B:18:ARG:HG3	1:B:197:GLU:HG3	2.01	0.42
3:D:170:LEU:HD13	3:D:209:ARG:NH2	2.34	0.42
3:D:139:VAL:HG11	3:D:231:PRO:HD3	2.01	0.42
3:D:369:ASN:ND2	5:F:260:GLN:OE1	2.50	0.42
7:J:106:LYS:CA	7:J:106:LYS:HE2	2.27	0.42
2:C:171:VAL:HG12	2:C:172:ARG:N	2.35	0.42
2:C:203:LEU:CD1	2:C:217:ILE:HB	2.50	0.42
2:C:623:LEU:HB3	2:C:703:GLU:HB3	2.02	0.42
2:C:70:GLU:N	2:C:70:GLU:OE1	2.53	0.42
3:D:1123:LEU:HB2	3:D:1131:VAL:HG21	2.02	0.42
3:D:248:TYR:HA	3:D:251:TYR:CD2	2.55	0.42
3:D:68:VAL:HG12	3:D:68:VAL:O	2.20	0.42
3:D:735:VAL:CG1	3:D:816:LEU:HD22	2.50	0.42
3:D:863:ALA:O	3:D:866:THR:HG22	2.20	0.42
3:D:900:LEU:C	3:D:900:LEU:HD23	2.40	0.42
3:D:934:ASN:O	3:D:935:VAL:C	2.57	0.42
4:E:30:LEU:N	4:E:30:LEU:HD12	2.35	0.42
5:F:320:ILE:HG23	5:F:340:GLU:CG	2.41	0.42
9:P:4:DA:H2"	9:P:5:DC:C6	2.55	0.42
1:B:105:VAL:HG12	1:B:125:ILE:CG2	2.49	0.42
1:B:22:VAL:HG12	1:B:193:ILE:CD1	2.50	0.42
1:B:66:VAL:HG12	1:B:69:VAL:HG22	2.01	0.42
1:B:32:TYR:CD1	2:C:1005:ARG:HD3	2.54	0.42
2:C:310:LYS:HE3	2:C:335:TYR:CE2	2.55	0.42
2:C:466:VAL:CG2	3:D:853:HIS:HA	2.50	0.42
2:C:509:LYS:HB3	2:C:569:TYR:CE2	2.54	0.42
2:C:716:PRO:HD3	2:C:910:THR:OG1	2.20	0.42
2:C:29:ARG:CG	2:C:964:ALA:HB2	2.49	0.42
4:E:26:TYR:O	4:E:27:ASP:CG	2.58	0.42
5:F:423:GLN:CG	5:F:425:ARG:HE	2.33	0.42
8:O:28:DT:H2'	8:O:29:DA:C8	2.54	0.42
1:A:107:ALA:HB1	1:A:118:VAL:HG11	2.02	0.41
1:B:183:VAL:HG13	3:D:488:GLU:CD	2.41	0.41
1:B:26:LEU:HD12	1:B:31:GLY:HA2	2.01	0.41
2:C:1003:ASP:HB2	2:C:1010:PHE:CE1	2.55	0.41
2:C:150:MET:CE	2:C:150:MET:HA	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:152:THR:HG21	2:C:158:ILE:HD11	2.02	0.41
2:C:795:GLY:HA2	2:C:827:SER:OG	2.20	0.41
2:C:875:LYS:C	2:C:876:LEU:HD12	2.40	0.41
2:C:980:LEU:HD13	2:C:980:LEU:HA	1.94	0.41
2:C:992:MET:HB3	2:C:992:MET:HE2	1.84	0.41
3:D:97:LEU:HA	3:D:351:ASN:OD1	2.19	0.41
5:F:338:ALA:HB2	5:F:348:VAL:CG1	2.49	0.41
1:A:11:GLU:CD	1:A:205:ARG:HG2	2.40	0.41
1:B:171:VAL:O	1:B:171:VAL:HG23	2.20	0.41
1:B:172:LEU:O	3:D:616:ALA:HB1	2.19	0.41
1:B:32:TYR:CZ	2:C:1005:ARG:NH1	2.88	0.41
2:C:235:THR:HG22	2:C:236:ASN:N	2.35	0.41
2:C:427:LEU:HD12	2:C:427:LEU:N	2.35	0.41
2:C:691:GLN:HG2	2:C:692:VAL:N	2.35	0.41
3:D:1031:ARG:NH2	3:D:1035:LEU:HD21	2.34	0.41
3:D:1054:VAL:HG12	3:D:1104:ASP:O	2.21	0.41
3:D:1112:LEU:HA	3:D:1112:LEU:HD12	1.87	0.41
3:D:1119:PRO:HA	3:D:1122:VAL:HG12	2.01	0.41
3:D:961:VAL:HG22	3:D:962:ARG:N	2.35	0.41
5:F:186:GLU:OE1	5:F:186:GLU:HA	2.21	0.41
5:F:438:ARG:NH1	9:P:20:DG:C5	2.83	0.41
2:C:1105:GLU:HG3	2:C:1106:PRO:HD2	2.03	0.41
2:C:202:TRP:H	2:C:202:TRP:HD1	1.68	0.41
2:C:236:ASN:HA	2:C:239:ILE:HD12	2.01	0.41
3:D:1266:SER:N	14:D:2012:GLU:N	2.66	0.41
3:D:527:LEU:HD21	3:D:581:MET:HE1	2.03	0.41
3:D:76:GLU:HA	7:J:44:PHE:CE2	2.48	0.41
3:D:748:HIS:CE1	3:D:780:ALA:HB2	2.55	0.41
3:D:822:LEU:HD23	3:D:834:PRO:CA	2.47	0.41
5:F:320:ILE:HG22	5:F:337:LEU:HD12	2.01	0.41
1:A:94:THR:HG22	1:A:139:VAL:HG22	2.02	0.41
1:B:99:LYS:HE2	1:B:99:LYS:HB3	1.75	0.41
2:C:763:ASP:HB3	2:C:821:ARG:NH2	2.24	0.41
3:D:636:ARG:HD3	3:D:660:ALA:HB1	2.01	0.41
3:D:742:GLN:O	3:D:746:GLU:HG2	2.20	0.41
3:D:904:GLY:HA3	3:D:910:ILE:HG22	2.02	0.41
5:F:201:LEU:CD2	5:F:211:LEU:HD11	2.50	0.41
5:F:324:LEU:CD2	5:F:332:PRO:HB3	2.32	0.41
7:J:98:LEU:HG	7:J:102:LEU:HD13	2.01	0.41
1:B:151:GLN:CG	1:B:151:GLN:O	2.68	0.41
2:C:573:SER:O	2:C:576:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:356:ARG:NH1	10:D:2010:SO4:O3	2.52	0.41
3:D:594:GLY:HA2	3:D:598:GLU:OE1	2.20	0.41
3:D:633:ILE:HD12	3:D:633:ILE:C	2.41	0.41
3:D:801:ILE:HG22	3:D:807:THR:O	2.20	0.41
3:D:904:GLY:HA3	3:D:910:ILE:HG21	2.02	0.41
8:O:15:DT:P	1:T:258:VAL:HG21	2.60	0.41
1:A:33:THR:HG22	1:B:37:SER:HA	2.03	0.41
2:C:1035:ARG:HD3	2:C:1056:GLY:CA	2.51	0.41
2:C:154:LYS:O	2:C:443:LYS:HE3	2.21	0.41
2:C:609:LEU:HD13	2:C:737:VAL:O	2.20	0.41
2:C:894:ASP:HA	2:C:1004:GLY:CA	2.48	0.41
3:D:1168:ILE:CD1	3:D:1176:PHE:HB3	2.45	0.41
2:C:1026:HIS:HB3	2:C:1031:LYS:CE	2.50	0.41
2:C:774:ASP:HA	2:C:782:ARG:HH21	1.86	0.41
2:C:76:GLY:O	2:C:80:VAL:HG23	2.21	0.41
2:C:870:ILE:HG23	2:C:870:ILE:O	2.20	0.41
3:D:1041:PRO:HB3	3:D:1116:ALA:CB	2.43	0.41
3:D:442:GLY:HA3	3:D:517:VAL:HG21	2.02	0.41
3:D:884:ILE:HD11	3:D:886:ARG:CD	2.50	0.41
1:A:120:ASN:N	1:A:121:PRO:HD3	2.36	0.41
1:A:50:ALA:HB3	1:A:168:TYR:CD1	2.56	0.41
2:C:246:SER:CB	2:C:337:VAL:HG11	2.51	0.41
2:C:94:MET:HE1	2:C:395:MET:HB3	1.99	0.41
2:C:53:GLU:O	2:C:57:GLY:N	2.51	0.41
2:C:935:TRP:HA	2:C:982:SER:HB3	2.02	0.41
2:C:926:HIS:CE1	2:C:997:GLY:HA3	2.56	0.41
3:D:110:VAL:HA	3:D:111:PRO:HA	1.91	0.41
3:D:190:LYS:NZ	3:D:192:ASP:CB	2.80	0.41
3:D:612:TYR:HB2	3:D:635:VAL:CG1	2.50	0.41
8:O:6:DA:H1'	8:O:7:DC:C5'	2.50	0.41
2:C:387:MET:O	2:C:391:VAL:HG23	2.20	0.41
2:C:427:LEU:HD12	2:C:427:LEU:H	1.85	0.41
2:C:461:LEU:N	2:C:461:LEU:HD23	2.36	0.41
2:C:714:ILE:HD13	2:C:922:ILE:HD12	2.03	0.41
3:D:1168:ILE:HD13	3:D:1176:PHE:CG	2.55	0.41
3:D:191:SER:HA	3:D:194:ARG:HE	1.85	0.41
3:D:47:PHE:HD1	3:D:322:PRO:HB3	1.86	0.41
3:D:738:PRO:HA	3:D:791:PHE:CD2	2.56	0.41
3:D:927:ASP:OD1	3:D:938:GLU:HA	2.21	0.41
3:D:885:VAL:O	3:D:990:ILE:O	2.38	0.41
5:F:174:GLY:HA2	5:F:239:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:246:LYS:HB3	5:F:246:LYS:HE2	1.84	0.41
1:B:137:GLU:HG2	1:B:138:LEU:N	2.36	0.41
1:B:17:ASN:OD1	1:B:17:ASN:N	2.40	0.41
2:C:265:LEU:CD2	2:C:284:GLN:HA	2.44	0.41
2:C:755:LEU:HD21	2:C:800:LYS:O	2.21	0.41
3:D:417:LEU:HD12	3:D:417:LEU:HA	1.77	0.41
3:D:706:ILE:CD1	4:E:36:PRO:HA	2.51	0.41
5:F:214:GLN:NE2	5:F:214:GLN:HA	2.35	0.41
1:B:200:ASN:ND2	1:B:200:ASN:H	2.18	0.41
2:C:540:ASP:O	2:C:543:GLY:N	2.46	0.41
2:C:744:GLU:HG3	2:C:834:GLU:OE2	2.21	0.41
3:D:190:LYS:CD	3:D:192:ASP:HB3	2.51	0.41
3:D:293:LEU:HD23	3:D:293:LEU:C	2.41	0.41
3:D:320:ILE:HG12	3:D:321:PRO:CD	2.49	0.41
5:F:283:THR:OG1	8:O:29:DA:H8	2.04	0.41
1:A:170:PRO:HB3	1:A:202:ILE:HG12	2.04	0.40
1:A:61:HIS:HD2	2:C:783:ILE:CD1	2.34	0.40
2:C:808:GLU:O	2:C:812:LEU:HD13	2.21	0.40
1:A:40:ARG:HH21	2:C:894:ASP:HB3	1.85	0.40
2:C:935:TRP:C	2:C:983:THR:HG23	2.42	0.40
3:D:1168:ILE:HD11	3:D:1182:THR:CG2	2.51	0.40
3:D:48:CYS:SG	3:D:51:ILE:HG13	2.61	0.40
5:F:201:LEU:HD21	5:F:211:LEU:HD11	2.03	0.40
5:F:309:HIS:O	5:F:313:VAL:HG12	2.21	0.40
5:F:313:VAL:HG21	5:F:351:ILE:HD13	2.03	0.40
1:A:27:GLU:HB3	1:A:28:PRO:HD2	2.02	0.40
2:C:728:LEU:HA	2:C:905:ASP:O	2.20	0.40
2:C:912:GLY:O	2:C:916:ARG:HG3	2.21	0.40
3:D:1045:ALA:HA	3:D:1046:PRO:HD3	1.89	0.40
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.96	0.40
3:D:603:THR:HG22	3:D:604:LYS:HE2	2.04	0.40
3:D:622:MET:HE1	3:D:629:VAL:HG13	2.03	0.40
5:F:267:ILE:O	5:F:271:GLU:HG3	2.21	0.40
5:F:451:LYS:O	5:F:454:HIS:HB3	2.21	0.40
7:J:58:ASN:HD21	7:J:60:LEU:CD1	2.34	0.40
1:A:11:GLU:OE2	1:B:225:LEU:HD22	2.22	0.40
2:C:199:ARG:HB3	2:C:199:ARG:NH1	2.36	0.40
2:C:798:THR:HG23	2:C:826:THR:OG1	2.21	0.40
2:C:852:LEU:HD23	2:C:856:VAL:HG12	2.03	0.40
2:C:727:ILE:CD1	2:C:907:ILE:HD12	2.49	0.40
3:D:736:LEU:HA	3:D:736:LEU:HD13	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:796:ASN:ND2	3:D:798:ILE:H	2.20	0.40
3:D:837:SER:HB2	3:D:847:GLU:OE1	2.21	0.40
4:E:80:VAL:CG2	4:E:100:LEU:HD22	2.52	0.40
2:C:1074:TYR:CE2	4:E:52:ILE:HD11	2.56	0.40
5:F:308:VAL:HG23	5:F:309:HIS:N	2.37	0.40
3:D:22:ASN:HA	7:J:57:ARG:HH12	1.86	0.40
8:O:11:DA:C2'	8:O:12:DG:H5''	2.51	0.40
1:B:106:THR:HA	1:B:123:MET:O	2.22	0.40
1:B:95:MET:HB3	1:B:110:ILE:HD11	2.02	0.40
1:B:134:LEU:HD23	1:B:134:LEU:C	2.42	0.40
1:B:19:SER:O	1:B:196:VAL:HG12	2.22	0.40
1:A:210:SER:CB	1:B:229:SER:HB3	2.49	0.40
2:C:1028:VAL:HG12	3:D:429:VAL:HG11	2.02	0.40
2:C:1105:GLU:HA	2:C:1106:PRO:HD3	1.97	0.40
2:C:203:LEU:O	2:C:204:GLU:HG3	2.21	0.40
2:C:597:LEU:HD23	2:C:597:LEU:C	2.42	0.40
2:C:748:ILE:HB	2:C:828:LEU:HD22	2.02	0.40
2:C:618:GLY:O	2:C:964:ALA:HA	2.21	0.40
3:D:784:VAL:O	3:D:788:LEU:HB2	2.21	0.40
5:F:317:LEU:HD21	5:F:337:LEU:CD2	2.51	0.40
1:B:113:PRO:O	1:B:116:VAL:HG22	2.21	0.40
2:C:1067:MET:HE2	2:C:1067:MET:HB2	1.87	0.40
2:C:123:PRO:HB3	2:C:144:PHE:HE1	1.86	0.40
2:C:204:GLU:N	2:C:216:ARG:O	2.47	0.40
2:C:479:THR:OG1	2:C:480:PRO:HD2	2.22	0.40
2:C:560:GLU:CG	2:C:561:PHE:N	2.85	0.40
2:C:614:ALA:CB	2:C:700:GLN:HE21	2.35	0.40
2:C:790:GLY:H	2:C:830:VAL:HG12	1.86	0.40
3:D:898:VAL:HG11	3:D:919:ALA:HB2	2.04	0.40
4:E:40:LEU:HB3	4:E:50:LEU:HD11	2.03	0.40
2:C:810:ARG:NH2	5:F:424:PRO:HG3	2.37	0.40
7:J:74:LYS:CD	7:J:74:LYS:O	2.69	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:658:ARG:NH1	3:D:147:GLU:OE1[2_356]	1.99	0.21

## 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	214/350 (61%)	204 (95%)	9 (4%)	1 (0%)	29	60
1	B	231/350 (66%)	211 (91%)	20 (9%)	0	100	100
1	T	51/350 (15%)	51 (100%)	0	0	100	100
2	C	1093/1169 (94%)	1040 (95%)	51 (5%)	2 (0%)	47	77
3	D	1234/1317 (94%)	1185 (96%)	45 (4%)	4 (0%)	41	70
4	E	72/107 (67%)	66 (92%)	5 (7%)	1 (1%)	11	36
5	F	303/466 (65%)	299 (99%)	4 (1%)	0	100	100
7	J	81/114 (71%)	77 (95%)	3 (4%)	1 (1%)	13	40
All	All	3279/4223 (78%)	3133 (96%)	137 (4%)	9 (0%)	41	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	931	ALA
3	D	1010	THR
2	C	325	THR
3	D	1086	ARG
2	C	850	ASP
3	D	932	ASN
4	E	27	ASP
1	A	91	GLU
7	J	70	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	174/297 (59%)	161 (92%)	13 (8%)	13	39
1	B	171/297 (58%)	158 (92%)	13 (8%)	13	38
1	T	26/297 (9%)	25 (96%)	1 (4%)	33	63
2	C	860/984 (87%)	798 (93%)	62 (7%)	14	40
3	D	989/1095 (90%)	913 (92%)	76 (8%)	13	38
4	E	62/86 (72%)	51 (82%)	11 (18%)	2	7
5	F	253/379 (67%)	236 (93%)	17 (7%)	16	43
7	J	72/98 (74%)	65 (90%)	7 (10%)	8	27
All	All	2607/3533 (74%)	2407 (92%)	200 (8%)	13	38

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	40	ARG
1	A	51	VAL
1	A	71	GLU
1	A	74	THR
1	A	127	THR
1	A	129	ASN
1	A	130	ASP
1	A	135	GLU
1	A	142	ARG
1	A	150	VAL
1	A	159	ILE
1	A	168	TYR
1	B	17	ASN
1	B	33	THR
1	B	60	LEU
1	B	84	VAL
1	B	125	ILE
1	B	144	ARG
1	B	161	ARG
1	B	176	TYR
1	B	185	GLN
1	B	200	ASN
1	B	215	LEU
1	B	230	GLU

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Mol	Chain	Res	Type
1	B	231	HIS
2	C	44	LEU
2	C	67	ASP
2	C	70	GLU
2	C	102	ARG
2	C	119	THR
2	C	124	LEU
2	C	202	TRP
2	C	215	VAL
2	C	236	ASN
2	C	273	ARG
2	C	294	GLU
2	C	299	LEU
2	C	301	ARG
2	C	323	THR
2	C	324	LEU
2	C	335	TYR
2	C	346	MET
2	C	398	GLN
2	C	437	LEU
2	C	447	SER
2	C	454	LEU
2	C	461	LEU
2	C	466	VAL
2	C	520	ASP
2	C	523	THR
2	C	525	ASP
2	C	534	GLN
2	C	545	PHE
2	C	546	THR
2	C	568	ASP
2	C	604	ARG
2	C	607	VAL
2	C	611	ARG
2	C	623	LEU
2	C	658	ARG
2	C	727	ILE
2	C	753	THR
2	C	763	ASP
2	C	771	VAL
2	C	775	LEU
2	C	777	GLU

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Mol	Chain	Res	Type
2	C	778	ARG
2	C	780	ILE
2	C	783	ILE
2	C	872	ASP
2	C	895	MET
2	C	919	ILE
2	C	927	LEU
2	C	936	ASN
2	C	945	ASP
2	C	954	LEU
2	C	965	THR
2	C	984	LEU
2	C	986	ASN
2	C	988	ASP
2	C	1022	LEU
2	C	1045	GLN
2	C	1048	LEU
2	C	1054	PHE
2	C	1108	ILE
2	C	1122	LEU
2	C	1138	MET
3	D	7	PHE
3	D	12	ILE
3	D	28	VAL
3	D	51	ILE
3	D	70	PHE
3	D	88	ARG
3	D	101	VAL
3	D	107	PHE
3	D	144	ARG
3	D	148	LEU
3	D	150	THR
3	D	165	GLN
3	D	187	GLU
3	D	238	GLU
3	D	239	VAL
3	D	243	GLU
3	D	246	ASP
3	D	281	ILE
3	D	295	ARG
3	D	298	VAL
3	D	314	LEU

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Mol	Chain	Res	Type
3	D	330	LEU
3	D	365	ILE
3	D	415	GLN
3	D	417	LEU
3	D	449	LEU
3	D	451	LEU
3	D	456	VAL
3	D	467	GLN
3	D	499	ASN
3	D	507	LEU
3	D	558	LEU
3	D	566	LEU
3	D	588	LEU
3	D	591	LEU
3	D	627	LEU
3	D	635	VAL
3	D	650	LEU
3	D	656	LYS
3	D	675	LEU
3	D	687	MET
3	D	724	THR
3	D	736	LEU
3	D	740	GLN
3	D	767	THR
3	D	779	ASP
3	D	784	VAL
3	D	791	PHE
3	D	799	ILE
3	D	830	PHE
3	D	831	ILE
3	D	841	GLU
3	D	846	LEU
3	D	853	HIS
3	D	862	THR
3	D	876	LEU
3	D	900	LEU
3	D	914	HIS
3	D	930	ASP
3	D	934	ASN
3	D	939	ARG
3	D	945	ASP
3	D	952	LEU

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Mol	Chain	Res	Type
3	D	1056	LEU
3	D	1063	PHE
3	D	1071	ASP
3	D	1079	ASP
3	D	1086	ARG
3	D	1110	ASP
3	D	1112	LEU
3	D	1183	GLU
3	D	1186	GLU
3	D	1190	GLU
3	D	1208	LEU
3	D	1222	LEU
3	D	1278	GLU
4	E	37	ILE
4	E	50	LEU
4	E	53	TYR
4	E	57	ARG
4	E	59	ARG
4	E	75	TYR
4	E	76	VAL
4	E	85	GLN
4	E	101	LEU
4	E	102	GLU
4	E	103	HIS
5	F	182	GLU
5	F	216	ARG
5	F	291	GLN
5	F	310	MET
5	F	313	VAL
5	F	348	VAL
5	F	349	LEU
5	F	365	ILE
5	F	367	ASP
5	F	372	GLN
5	F	407	GLU
5	F	423	GLN
5	F	433	VAL
5	F	452	LEU
5	F	462	ARG
5	F	465	LEU
5	F	466	ASP
7	J	47	ASP

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Mol	Chain	Res	Type
7	J	55	LEU
7	J	64	LEU
7	J	74	LYS
7	J	92	GLU
7	J	104	LEU
7	J	105	ILE
1	T	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	124	HIS
1	A	129	ASN
1	B	124	HIS
1	B	185	GLN
2	C	48	GLN
2	C	160	ASN
2	C	343	GLN
2	C	398	GLN
2	C	433	GLN
2	C	576	GLN
2	C	590	HIS
2	C	603	GLN
2	C	700	GLN
2	C	720	HIS
2	C	721	ASN
2	C	911	HIS
2	C	936	ASN
3	D	165	GLN
3	D	287	GLN
3	D	303	GLN
3	D	416	ASN
3	D	465	HIS
3	D	494	HIS
3	D	499	ASN
3	D	515	GLN
3	D	564	ASN
3	D	600	GLN
3	D	684	ASN
3	D	692	GLN
3	D	740	GLN

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Mol	Chain	Res	Type
3	D	748	HIS
3	D	778	GLN
3	D	796	ASN
3	D	881	GLN
3	D	888	HIS
3	D	932	ASN
3	D	1085	GLN
3	D	1126	GLN
3	D	1140	GLN
3	D	1146	GLN
4	E	62	ASN
4	E	85	GLN
4	E	103	HIS
5	F	214	GLN
5	F	321	GLN
5	F	372	GLN
5	F	397	GLN
5	F	454	HIS
7	J	58	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	$\# Z  > 2$
11	EDO	F	506	-	3,3,3	0.46	0	2,2,2	0.27	0
11	EDO	C	1207	-	3,3,3	0.44	0	2,2,2	0.32	0
12	RFP	C	1205	-	63,63,63	2.64	17 (26%)	94,94,94	1.93	19 (20%)
11	EDO	D	2007	-	3,3,3	0.45	0	2,2,2	0.30	0
11	EDO	D	2009	-	3,3,3	0.47	0	2,2,2	0.26	0
10	SO4	D	2004	-	4,4,4	0.13	0	6,6,6	0.06	0
10	SO4	D	2003	-	4,4,4	0.14	0	6,6,6	0.07	0
11	EDO	D	2011	-	3,3,3	0.45	0	2,2,2	0.26	0
10	SO4	D	2005	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	C	1202	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	D	2006	-	4,4,4	0.14	0	6,6,6	0.05	0
14	GLU	D	2012	-	4,8,9	0.61	0	1,9,11	0.12	0
10	SO4	F	501	5	4,4,4	0.13	0	6,6,6	0.04	0
10	SO4	C	1201	-	4,4,4	0.14	0	6,6,6	0.05	0
11	EDO	C	1204	-	3,3,3	0.43	0	2,2,2	0.42	0
11	EDO	D	2008	-	3,3,3	0.45	0	2,2,2	0.31	0
11	EDO	F	505	-	3,3,3	0.46	0	2,2,2	0.26	0
10	SO4	F	503	-	4,4,4	0.14	0	6,6,6	0.06	0
10	SO4	F	504	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	C	1203	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.05	0
10	SO4	D	2010	-	4,4,4	0.14	0	6,6,6	0.04	0
10	SO4	C	1206	-	4,4,4	0.15	0	6,6,6	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	D	2009	-	-	1/1/1/1	-
11	EDO	F	506	-	-	1/1/1/1	-
11	EDO	C	1207	-	-	0/1/1/1	-
11	EDO	D	2007	-	-	0/1/1/1	-
11	EDO	D	2011	-	-	1/1/1/1	-
12	RFP	C	1205	-	-	13/60/85/85	0/5/5/5
11	EDO	C	1204	-	-	1/1/1/1	-
14	GLU	D	2012	-	-	1/4/7/9	-
11	EDO	D	2008	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	EDO	F	505	-	-	1/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	1205	RFP	C17-C16	8.22	1.58	1.34
12	C	1205	RFP	C15-N1	7.10	1.50	1.35
12	C	1205	RFP	C1-C9	6.55	1.63	1.43
12	C	1205	RFP	C18-C19	6.42	1.59	1.33
12	C	1205	RFP	C29-C28	5.85	1.60	1.30
12	C	1205	RFP	O3-C6	5.54	1.48	1.37
12	C	1205	RFP	C18-C17	4.96	1.58	1.43
12	C	1205	RFP	C2-N1	4.76	1.52	1.43
12	C	1205	RFP	C3-C43	4.56	1.55	1.46
12	C	1205	RFP	C12-C11	-3.47	1.40	1.54
12	C	1205	RFP	O5-C29	3.28	1.47	1.39
12	C	1205	RFP	O7-C35	3.27	1.42	1.35
12	C	1205	RFP	O7-C25	-2.73	1.40	1.44
12	C	1205	RFP	C6-C7	2.33	1.43	1.39
12	C	1205	RFP	C5-C11	2.32	1.52	1.41
12	C	1205	RFP	N3-N2	2.23	1.44	1.39
12	C	1205	RFP	O11-C15	-2.19	1.19	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	1205	RFP	C2-C3-C43	-6.94	117.11	124.17
12	C	1205	RFP	C2-C3-C4	6.63	123.46	119.20
12	C	1205	RFP	O3-C6-C7	6.10	131.63	121.14
12	C	1205	RFP	O7-C35-C36	5.18	120.61	111.09
12	C	1205	RFP	C20-C21-C22	-3.52	107.80	114.96
12	C	1205	RFP	C24-C23-C22	-3.47	109.62	115.43
12	C	1205	RFP	C40-C39-N4	3.42	114.67	110.80
12	C	1205	RFP	C41-C42-N4	2.98	114.17	110.80
12	C	1205	RFP	O4-C11-C12	2.79	126.24	120.56
12	C	1205	RFP	C25-O7-C35	-2.78	113.42	117.72
12	C	1205	RFP	O4-C11-C5	-2.69	126.68	131.81
12	C	1205	RFP	C20-C19-C18	-2.65	120.59	126.16
12	C	1205	RFP	C3-C2-N1	2.55	123.49	119.25
12	C	1205	RFP	C30-C16-C15	2.52	121.65	115.28
12	C	1205	RFP	C4-C3-C43	2.43	119.43	116.52
12	C	1205	RFP	O3-C12-C11	2.33	108.38	104.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	1205	RFP	C39-C40-N3	2.15	114.01	110.51
12	C	1205	RFP	O3-C6-C5	-2.10	107.75	113.57
12	C	1205	RFP	C16-C15-N1	-2.09	108.71	116.11

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	1205	RFP	C4-C3-C43-N2
12	C	1205	RFP	C13-C12-O5-C29
12	C	1205	RFP	C26-C27-C28-C29
12	C	1205	RFP	O6-C27-C28-C29
12	C	1205	RFP	C43-N2-N3-C40
11	D	2011	EDO	O1-C1-C2-O2
12	C	1205	RFP	C3-C2-N1-C15
12	C	1205	RFP	O3-C12-O5-C29
11	F	505	EDO	O1-C1-C2-O2
12	C	1205	RFP	C11-C12-O5-C29
12	C	1205	RFP	C33-C24-C25-C26
11	C	1204	EDO	O1-C1-C2-O2
12	C	1205	RFP	C2-C3-C43-N2
11	F	506	EDO	O1-C1-C2-O2
11	D	2009	EDO	O1-C1-C2-O2
12	C	1205	RFP	C33-C24-C25-O7
12	C	1205	RFP	C18-C19-C20-C31
14	D	2012	GLU	N-CA-CB-CG
12	C	1205	RFP	C31-C20-C21-C22

There are no ring outliers.

11 monomers are involved in 31 short contacts:

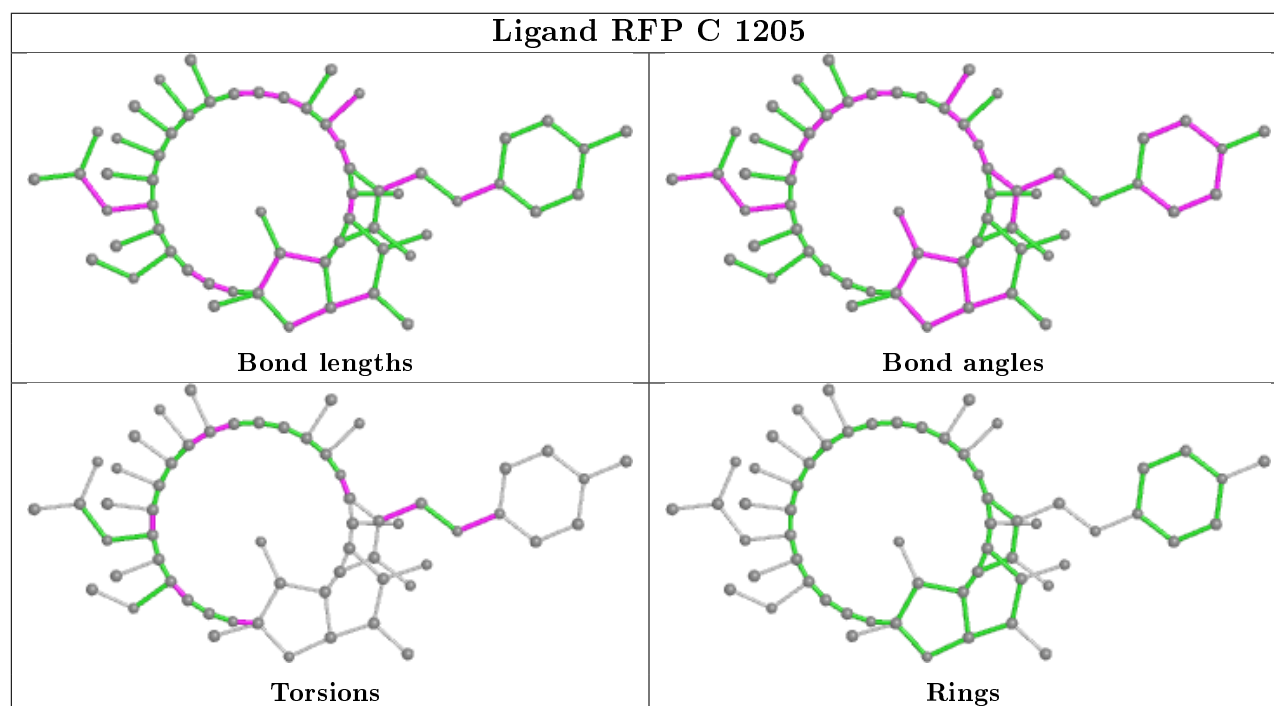
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	506	EDO	3	0
12	C	1205	RFP	9	0
11	D	2007	EDO	1	0
10	D	2004	SO4	2	0
11	D	2011	EDO	2	0
14	D	2012	GLU	10	0
10	C	1201	SO4	1	0
10	C	1203	SO4	1	0
10	F	502	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	D	2010	SO4	1	0
10	C	1206	SO4	1	0

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



## 5.7 Other polymers ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	218/350 (62%)	-0.27	0 <span>100</span> <span>100</span>	68, 97, 128, 146	0
1	B	233/350 (66%)	-0.00	5 (2%) <span>63</span> <span>39</span>	85, 121, 145, 161	0
1	T	53/350 (15%)	1.19	9 (16%) <span>1</span> <span>0</span>	123, 159, 184, 195	0
2	C	1099/1169 (94%)	-0.07	17 (1%) <span>73</span> <span>51</span>	47, 93, 154, 176	0
3	D	1246/1317 (94%)	-0.21	4 (0%) <span>94</span> <span>85</span>	41, 84, 140, 168	0
4	E	76/107 (71%)	-0.13	0 <span>100</span> <span>100</span>	61, 89, 131, 144	0
5	F	305/466 (65%)	-0.37	2 (0%) <span>87</span> <span>72</span>	46, 86, 135, 170	0
6	G	0/17	-	-	-	-
7	J	83/114 (72%)	-0.11	2 (2%) <span>59</span> <span>34</span>	70, 111, 158, 173	0
8	O	31/31 (100%)	-0.89	0 <span>100</span> <span>100</span>	59, 73, 96, 100	0
9	P	26/26 (100%)	-0.94	0 <span>100</span> <span>100</span>	66, 80, 94, 104	0
All	All	3370/4297 (78%)	-0.16	39 (1%) <span>79</span> <span>58</span>	41, 92, 150, 195	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	455	SER	7.0
1	B	1	MET	3.8
2	C	354	VAL	3.5
2	C	352	VAL	3.4
2	C	185	SER	3.1
2	C	950	LEU	3.1
7	J	74	LYS	3.0
2	C	550	VAL	2.9
2	C	228	LEU	2.9
2	C	181	THR	2.8
1	T	279	THR	2.8
2	C	350	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	738	PRO	2.7
3	D	1181	LEU	2.6
3	D	933	GLY	2.6
2	C	351	GLY	2.6
1	B	184	GLU	2.6
5	F	329	GLY	2.6
2	C	132	ASN	2.5
1	T	253	ASP	2.5
1	T	263	CYS	2.5
1	T	273	GLY	2.5
1	T	297	VAL	2.5
1	T	293	SER	2.5
1	T	267	GLU	2.5
2	C	189	THR	2.4
2	C	456	ARG	2.4
7	J	75	VAL	2.4
2	C	332	THR	2.3
1	B	183	VAL	2.3
2	C	353	GLU	2.3
3	D	186	ALA	2.2
5	F	215	GLN	2.2
1	B	3	ILE	2.2
1	T	269	VAL	2.2
2	C	459	ALA	2.2
1	T	302	HIS	2.2
1	B	21	PHE	2.1
2	C	302	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [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,



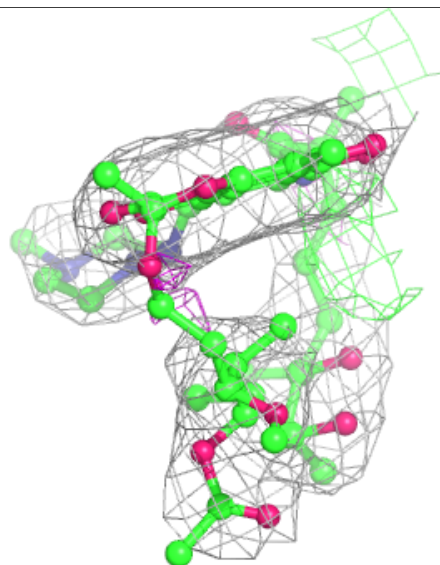
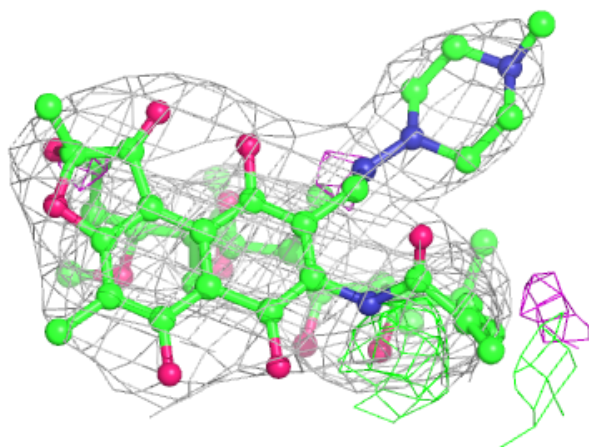
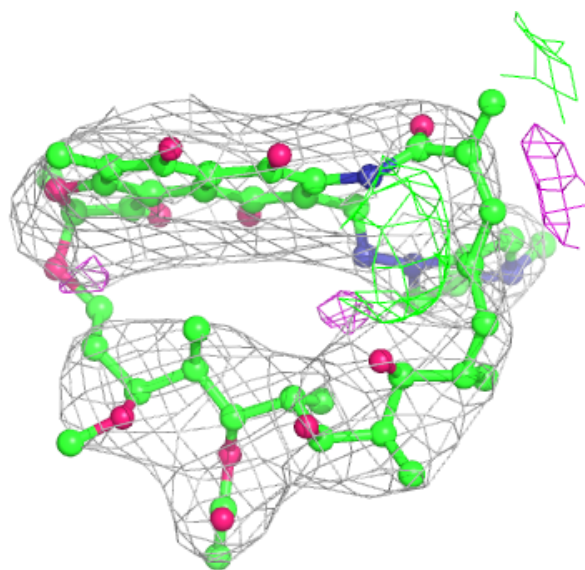
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	GLU	D	2012	9/10	0.71	0.30	90,97,100,110	0
10	SO4	C	1206	5/5	0.76	0.35	105,119,155,236	0
11	EDO	F	506	4/4	0.77	0.69	110,132,156,188	0
11	EDO	D	2007	4/4	0.82	0.28	75,94,113,123	0
10	SO4	D	2010	5/5	0.83	0.35	116,117,152,170	0
11	EDO	D	2011	4/4	0.86	0.24	73,87,105,105	0
10	SO4	C	1203	5/5	0.86	0.29	114,127,160,168	0
11	EDO	F	505	4/4	0.87	0.32	81,97,121,121	0
10	SO4	D	2006	5/5	0.87	0.25	116,124,133,140	0
10	SO4	D	2005	5/5	0.89	0.36	97,122,136,138	0
10	SO4	C	1202	5/5	0.89	0.16	119,126,141,149	0
11	EDO	D	2008	4/4	0.90	0.20	89,107,111,117	0
11	EDO	C	1207	4/4	0.90	0.28	94,113,134,134	0
10	SO4	F	504	5/5	0.90	0.11	121,127,136,142	0
10	SO4	F	503	5/5	0.91	0.12	104,110,129,130	0
10	SO4	D	2004	5/5	0.93	0.16	87,91,121,132	0
12	RFP	C	1205	59/59	0.94	0.24	47,69,104,119	0
10	SO4	C	1201	5/5	0.95	0.19	101,114,125,135	0
11	EDO	C	1204	4/4	0.95	0.26	61,74,92,92	0
11	EDO	D	2009	4/4	0.95	0.24	65,87,104,104	0
10	SO4	D	2003	5/5	0.96	0.22	64,76,98,102	0
13	ZN	D	2002	1/1	0.97	0.24	120,120,120,120	0
10	SO4	F	501	5/5	0.98	0.04	104,105,128,134	0
10	SO4	F	502	5/5	0.98	0.18	79,101,117,120	0
13	ZN	D	2001	1/1	0.98	0.33	129,129,129,129	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around RFP C 1205:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.