Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:34 PM GMT

PDB ID	:	4TMA
Title	:	Crystal structure of gyrase bound to its inhibitor YacG
Authors	:	Vos, S.M.; Lyubimov, A.Y.; Hershey, D.M.; Schoeffler, A.J.; Berger, J.M.
Deposited on	:	2014-05-31
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

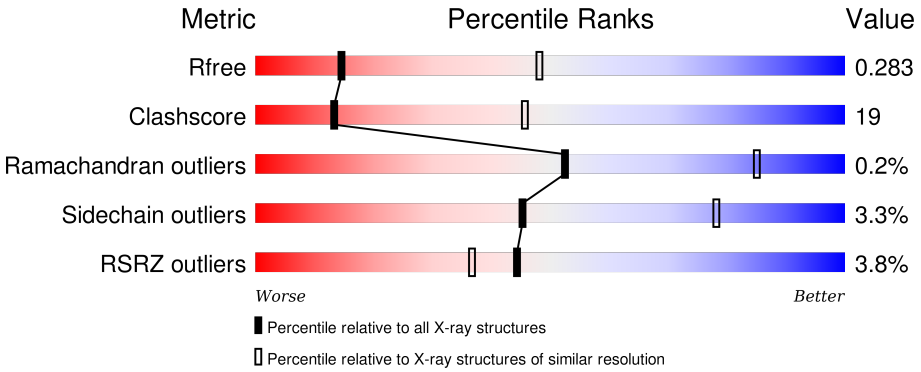
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	525	3% 58% 34%
1	C	525	5% 57% 31% 10%
1	E	525	3% 67% 25% 7%
1	G	525	3% 65% 25% 8%
2	B	417	% 53% 32% 10%

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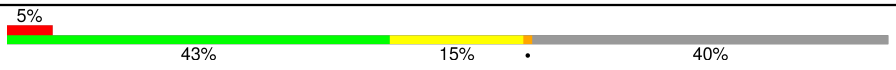
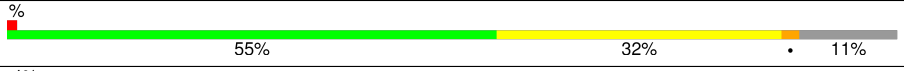
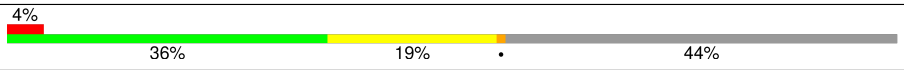
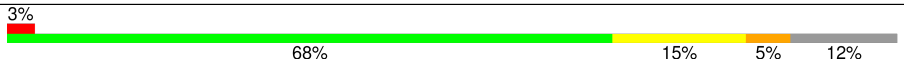
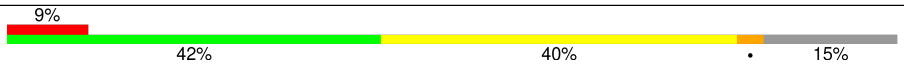
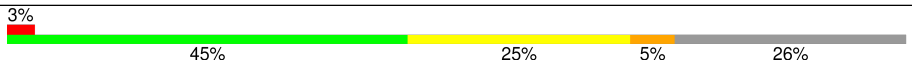
Mol	Chain	Length	Quality of chain
2	D	417	
2	F	417	
2	H	417	
3	I	65	
3	J	65	
3	K	65	
3	L	65	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26792 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	505	Total	C	N	O	S	0	0	0
			3983	2510	711	747	15			
1	C	475	Total	C	N	O	S	0	0	0
			3733	2345	672	701	15			
1	E	486	Total	C	N	O	S	0	1	0
			3841	2413	698	715	15			
1	G	483	Total	C	N	O	S	0	0	0
			3800	2391	682	713	14			

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	374	Total	C	N	O	S	0	0	0
			2995	1875	527	579	14			
2	D	251	Total	C	N	O	S	0	0	0
			1990	1252	347	379	12			
2	F	371	Total	C	N	O	S	0	0	0
			2971	1863	523	571	14			
2	H	233	Total	C	N	O	S	0	1	0
			1863	1170	326	356	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	385	SER	-	expression tag	UNP U6NGU8
B	386	ASN	-	expression tag	UNP U6NGU8
B	387	ALA	-	expression tag	UNP U6NGU8
B	458	TYR	PHE	engineered mutation	UNP U6NGU8
D	385	SER	-	expression tag	UNP U6NGU8
D	386	ASN	-	expression tag	UNP U6NGU8
D	387	ALA	-	expression tag	UNP U6NGU8
D	458	TYR	PHE	engineered mutation	UNP U6NGU8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	385	SER	-	expression tag	UNP U6NGU8
F	386	ASN	-	expression tag	UNP U6NGU8
F	387	ALA	-	expression tag	UNP U6NGU8
F	458	TYR	PHE	engineered mutation	UNP U6NGU8
H	385	SER	-	expression tag	UNP U6NGU8
H	386	ASN	-	expression tag	UNP U6NGU8
H	387	ALA	-	expression tag	UNP U6NGU8
H	458	TYR	PHE	engineered mutation	UNP U6NGU8

- Molecule 3 is a protein called DNA gyrase inhibitor YacG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	47	Total	C	N	O	S	0	0	0
			363	230	63	66	4			
3	J	57	Total	C	N	O	S	0	0	0
			446	279	74	89	4			
3	K	55	Total	C	N	O	S	0	0	0
			430	270	72	84	4			
3	L	48	Total	C	N	O	S	0	0	0
			371	234	64	69	4			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

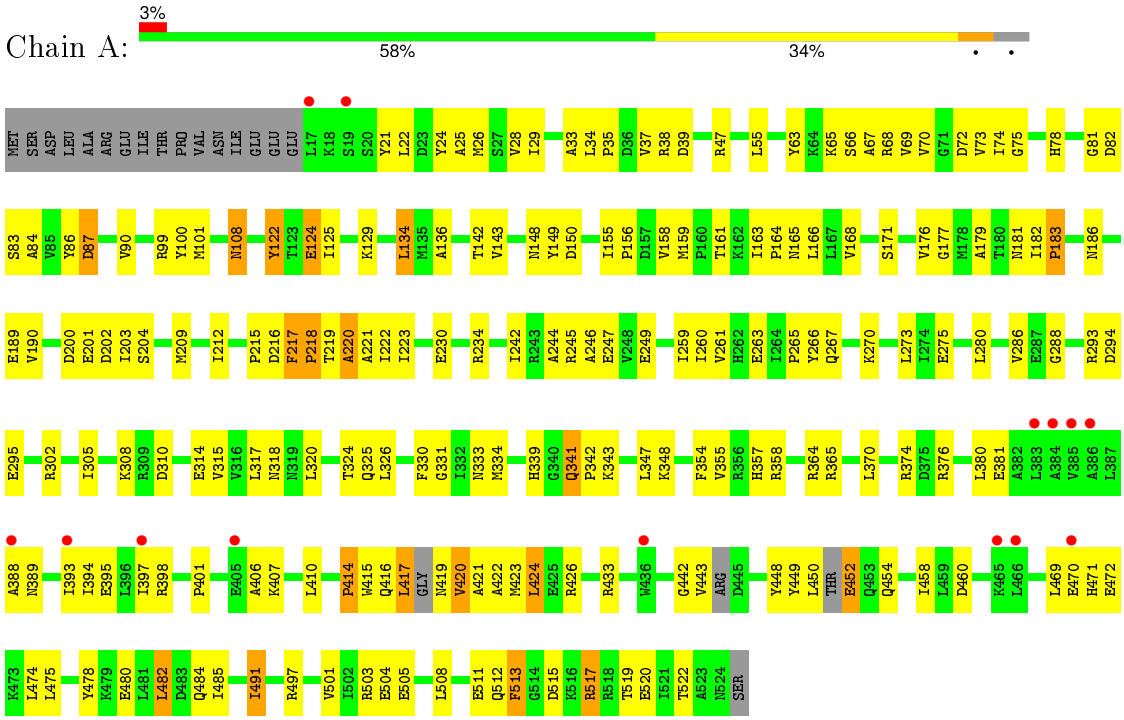
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	K	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		
4	L	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

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

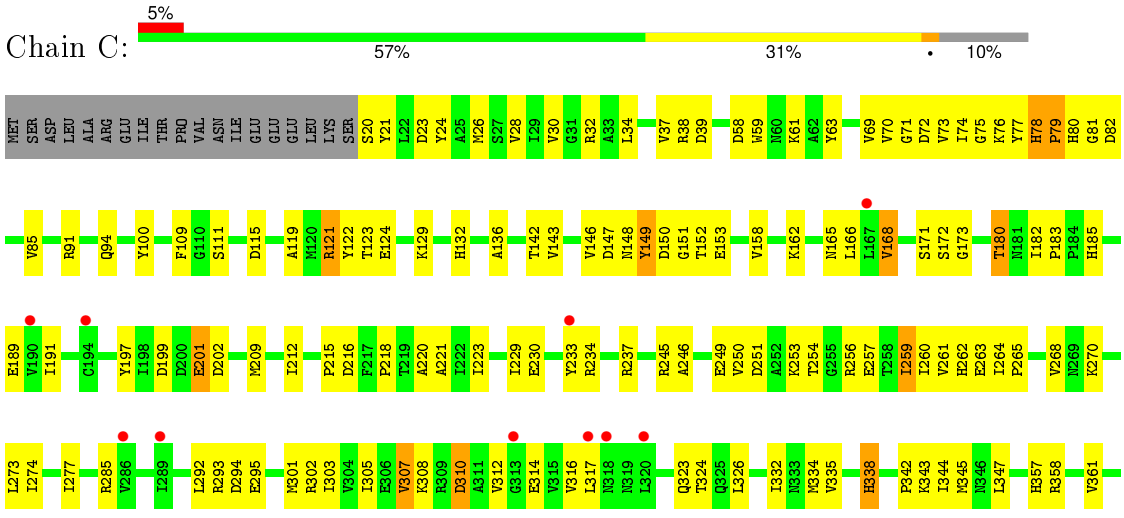
- Molecule 1: DNA gyrase subunit A

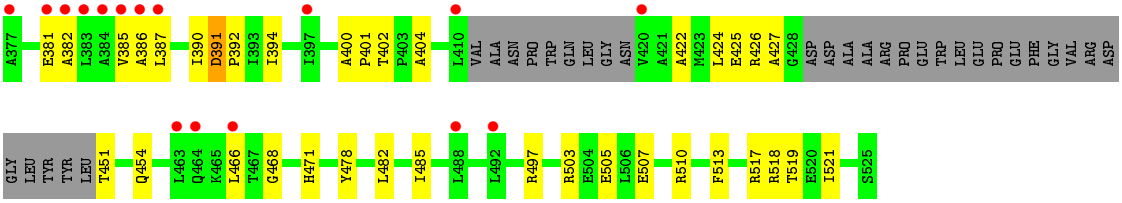
Chain A:

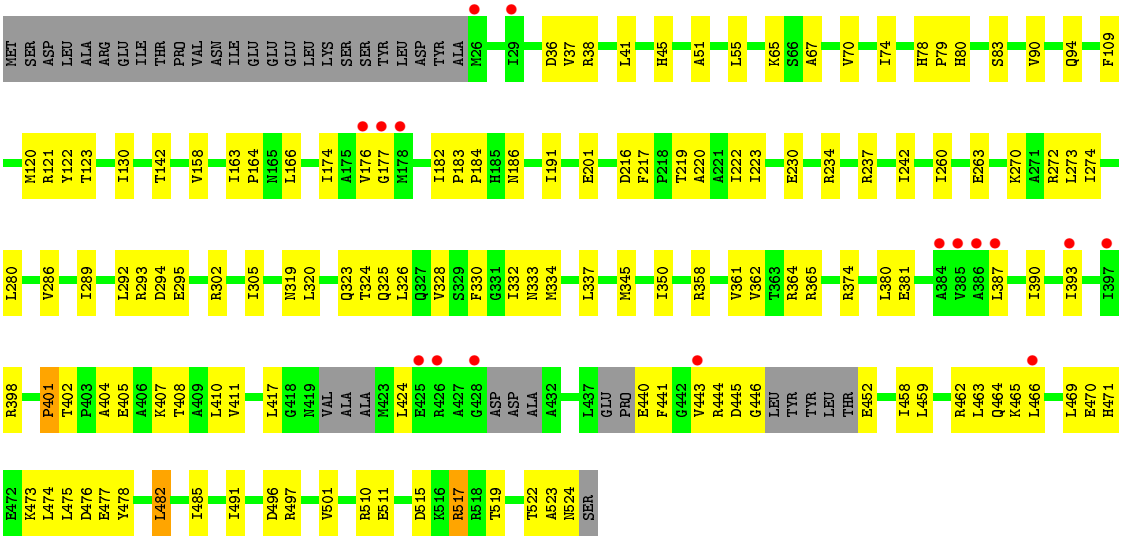


- Molecule 1: DNA gyrase subunit A

Chain C:





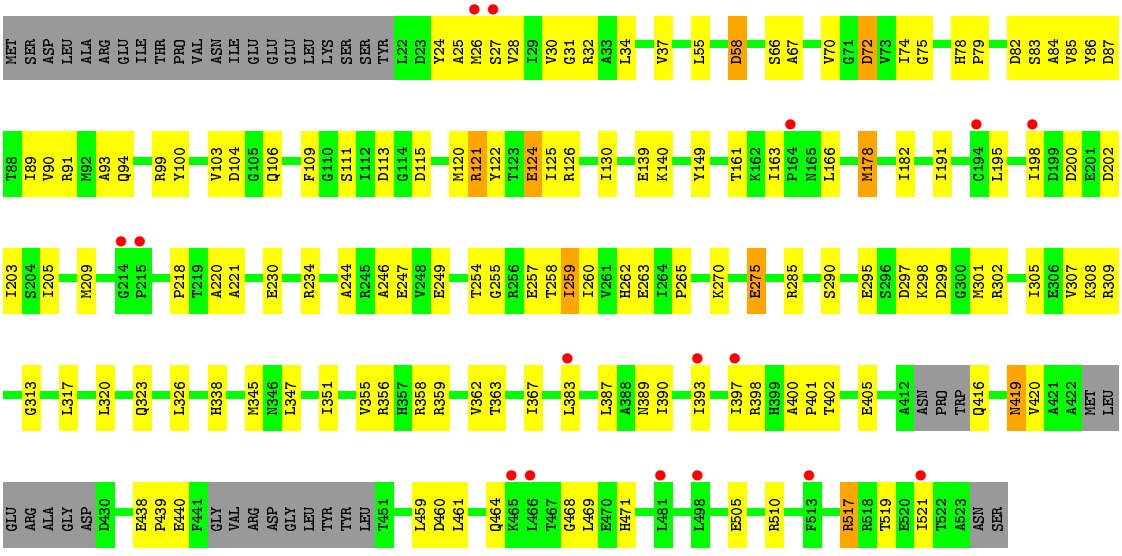


• Molecule 1: DNA gyrase subunit A

Chain E:

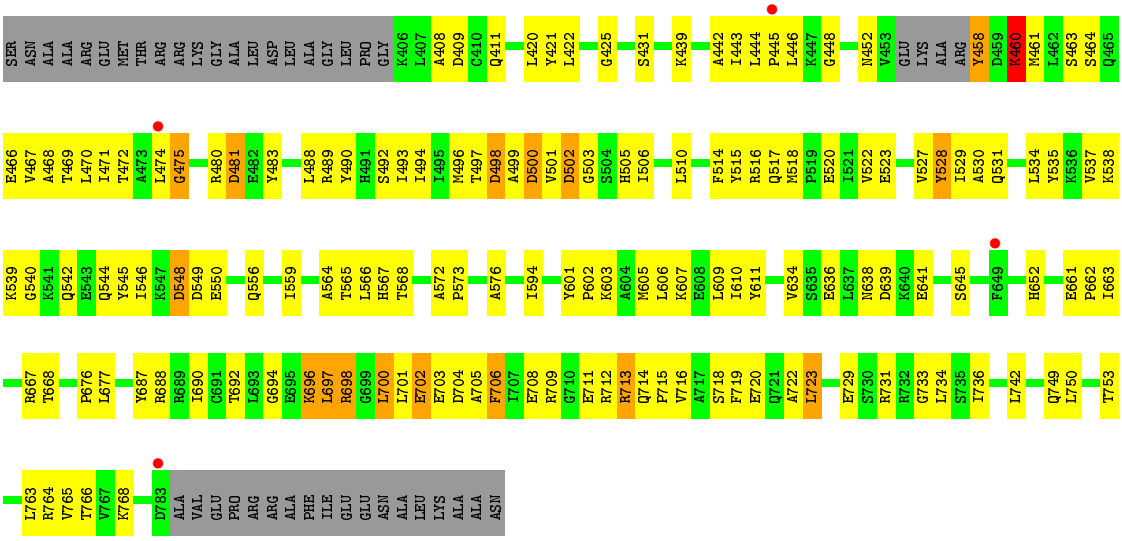
• Molecule 1: DNA gyrase subunit A

Chain G:



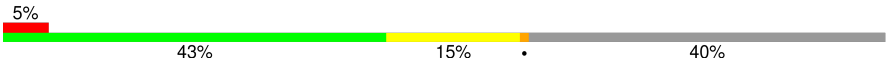
• Molecule 2: DNA gyrase subunit B

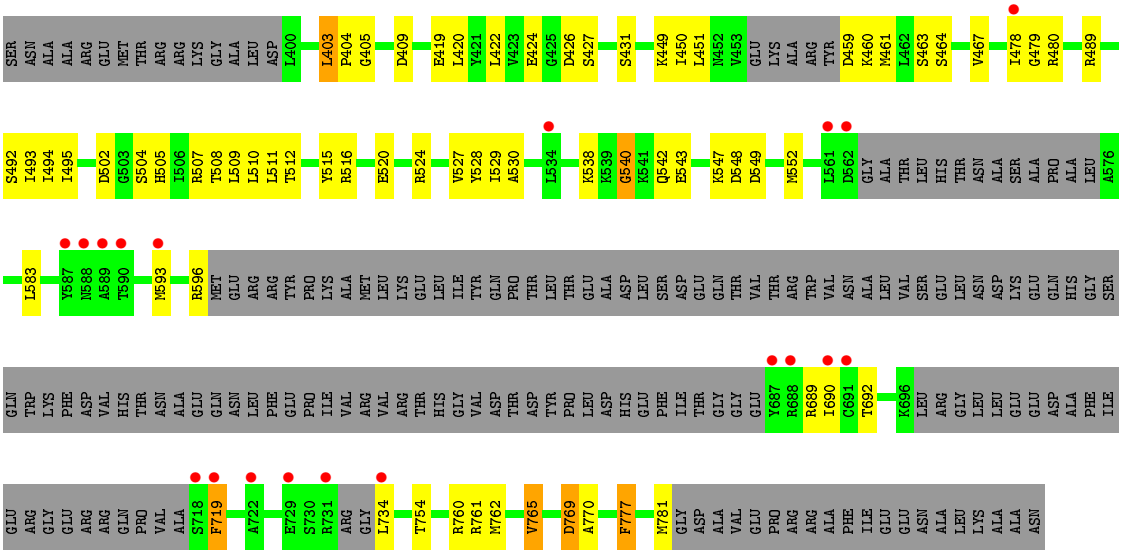
Chain B:



• Molecule 2: DNA gyrase subunit B

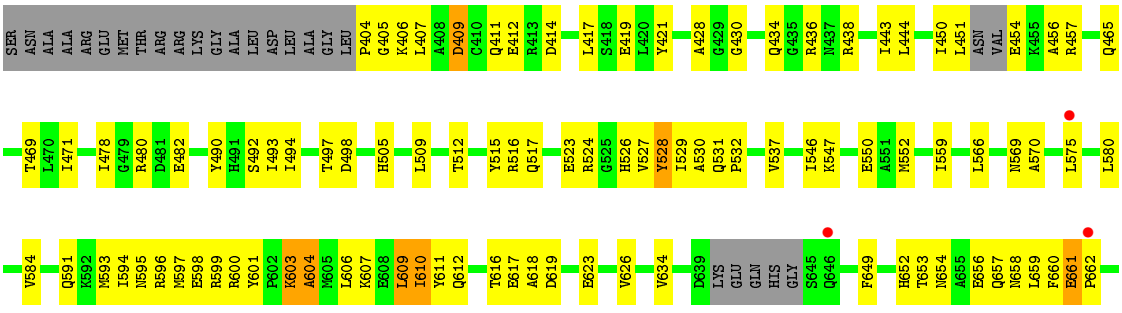
Chain D:

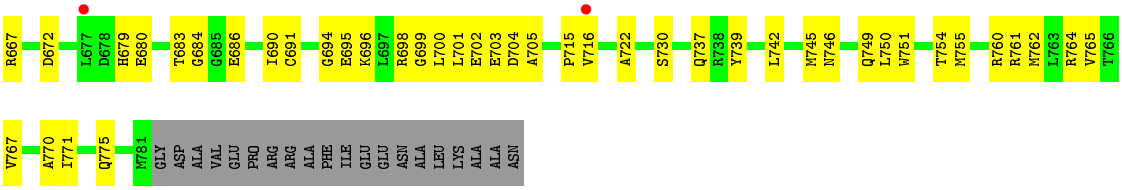




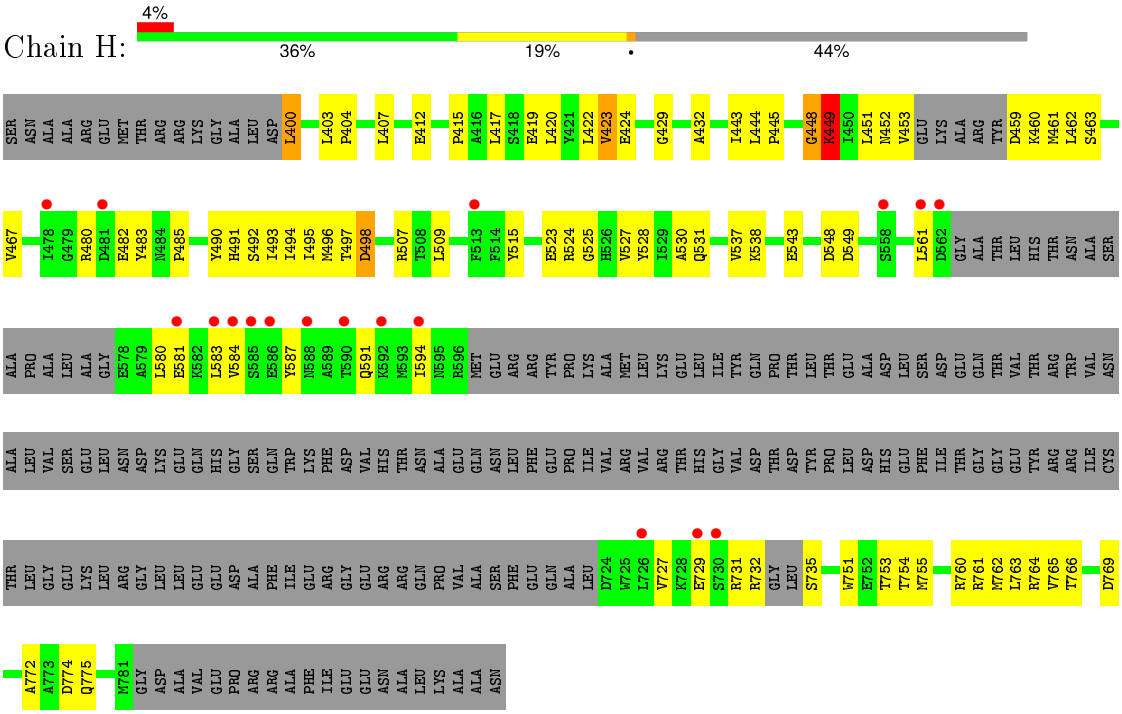
• Molecule 2: DNA gyrase subunit B

Chain F:

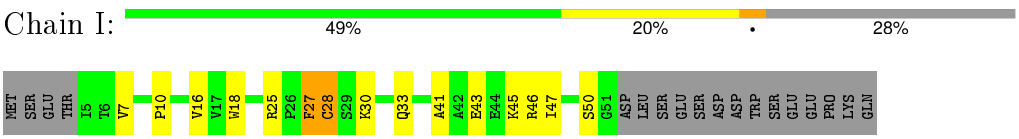




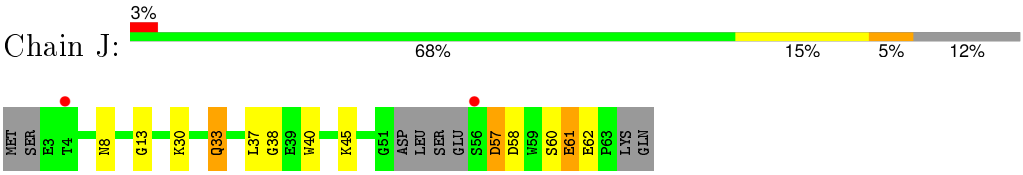
• Molecule 2: DNA gyrase subunit B



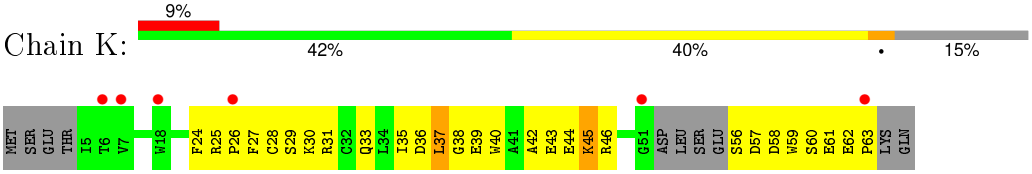
• Molecule 3: DNA gyrase inhibitor YacG



• Molecule 3: DNA gyrase inhibitor YacG

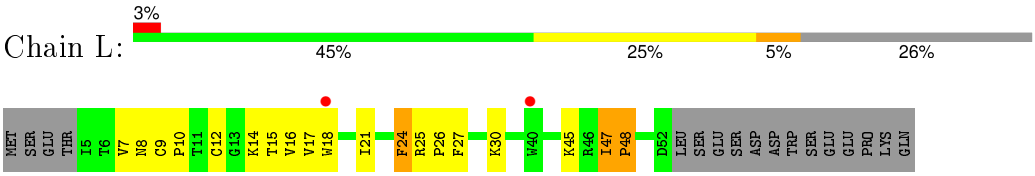


• Molecule 3: DNA gyrase inhibitor YacG



• Molecule 3: DNA gyrase inhibitor YacG

Chain L:


3%
45%
25%
5%
26%
MET SER GLU THR I5 T6 V7 N8 C9 P10 T11 C12 G13 K14 T15 V16 V17 W18 I21 F24 R25 P26 F27 K30 W40 K45 R46 I47 P48 D52 LEU SER GLU SER ASP ASP TRP SER GLU GLU PRO LYS GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.21Å 114.46Å 462.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.30 49.32 – 3.30	Depositor EDS
% Data completeness (in resolution range)	77.7 (49.32-3.30) 77.7 (49.32-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.243 , 0.283 0.243 , 0.283	Depositor DCC
R_{free} test set	3398 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	109.9	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 61.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 67314 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	26792	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.60	2/4044 (0.0%)	0.71	12/5466 (0.2%)
1	C	0.44	0/3785	0.61	4/5111 (0.1%)
1	E	0.47	0/3896	0.57	2/5258 (0.0%)
1	G	0.40	0/3855	0.51	1/5209 (0.0%)
2	B	0.47	1/3046 (0.0%)	0.73	8/4111 (0.2%)
2	D	0.37	0/2015	0.57	0/2705
2	F	0.40	0/3021	0.66	7/4074 (0.2%)
2	H	0.43	0/1887	0.66	4/2534 (0.2%)
3	I	0.65	0/372	0.92	4/504 (0.8%)
3	J	0.35	0/457	0.67	2/620 (0.3%)
3	K	0.81	1/441 (0.2%)	0.63	1/598 (0.2%)
3	L	0.73	2/380 (0.5%)	0.73	1/515 (0.2%)
All	All	0.47	6/27199 (0.0%)	0.64	46/36705 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	1
2	H	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	63	PRO	N-CD	-15.54	1.26	1.47
3	L	26	PRO	N-CD	9.27	1.60	1.47
3	L	48	PRO	N-CD	5.42	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	ASP	CA-C	5.37	1.67	1.52
1	A	218	PRO	N-CD	5.17	1.55	1.47
1	A	122	TYR	CE1-CZ	-5.00	1.32	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	28	CYS	O-C-N	-9.19	107.99	122.70
2	B	475	GLY	N-CA-C	8.69	134.84	113.10
1	A	419	ASN	N-CA-C	8.50	133.96	111.00
2	F	603	LYS	N-CA-C	8.06	132.76	111.00
3	I	47	ILE	CB-CA-C	-7.48	96.64	111.60
1	A	414	PRO	CB-CA-C	-7.24	93.91	112.00
1	A	417	LEU	N-CA-CB	-7.23	95.93	110.40
3	J	62	GLU	N-CA-CB	7.07	123.32	110.60
2	B	458	TYR	N-CA-C	6.83	129.44	111.00
1	C	148	ASN	CB-CA-C	6.77	123.94	110.40
1	A	420	VAL	N-CA-C	6.58	128.77	111.00
2	H	460	LYS	N-CA-C	6.53	128.64	111.00
1	A	419	ASN	CB-CA-C	6.30	123.00	110.40
2	B	697	LEU	N-CA-C	6.29	127.97	111.00
1	C	307	VAL	N-CA-C	6.28	127.94	111.00
1	A	183	PRO	C-N-CD	6.15	141.31	128.40
1	C	78	HIS	C-N-CD	6.02	141.05	128.40
2	B	460	LYS	N-CA-C	6.01	127.24	111.00
3	K	63	PRO	N-CD-CG	5.96	112.15	103.20
3	I	28	CYS	CA-C-N	5.93	130.24	117.20
2	F	528	TYR	C-N-CA	5.91	136.47	121.70
2	F	604	ALA	N-CA-CB	-5.90	101.84	110.10
1	A	339	HIS	CB-CA-C	-5.86	98.68	110.40
1	A	452	GLU	N-CA-C	5.85	126.78	111.00
2	F	604	ALA	N-CA-C	5.83	126.75	111.00
3	J	61	GLU	CB-CA-C	-5.76	98.89	110.40
1	C	259	ILE	CB-CA-C	-5.75	100.10	111.60
1	E	452	GLU	N-CA-C	5.74	126.51	111.00
1	A	419	ASN	N-CA-CB	-5.74	100.28	110.60
2	F	456	ALA	N-CA-CB	-5.71	102.11	110.10
1	A	217	PHE	C-N-CD	5.61	140.18	128.40
1	G	259	ILE	N-CA-C	-5.57	95.97	111.00
3	I	27	PHE	O-C-N	-5.54	113.84	122.70
1	A	452	GLU	N-CA-CB	-5.53	100.65	110.60
3	L	47	ILE	C-N-CD	5.52	140.00	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	424	LEU	N-CA-CB	5.45	121.29	110.40
2	H	448	GLY	N-CA-C	5.44	126.69	113.10
2	B	698	ARG	CB-CA-C	-5.39	99.62	110.40
2	H	400	LEU	CA-CB-CG	5.37	127.66	115.30
2	F	451	LEU	CA-CB-CG	5.35	127.61	115.30
1	E	219	THR	CB-CA-C	-5.35	97.16	111.60
2	B	713	ARG	N-CA-CB	-5.33	101.01	110.60
2	H	449	LYS	N-CA-C	5.31	125.34	111.00
2	F	528	TYR	O-C-N	5.22	131.05	122.70
2	B	502	ASP	CA-C-N	-5.20	105.81	116.20
2	B	700	LEU	N-CA-C	5.01	124.54	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	251	ASP	Peptide
2	D	540	GLY	Peptide
2	H	449	LYS	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	3983	0	4040	184	1
1	C	3733	0	3810	152	1
1	E	3841	0	3910	120	14
1	G	3800	0	3867	106	0
2	B	2995	0	2972	159	1
2	D	1990	0	2013	83	0
2	F	2971	0	2959	128	14
2	H	1863	0	1887	69	1
3	I	363	0	357	17	0
3	J	446	0	416	11	0
3	K	430	0	404	38	0
3	L	371	0	362	18	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
All	All	26792	0	26997	1011	16

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 19.

All (1011) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:760:ARG:HD3	2:D:762:MET:CE	1.40	1.52
1:G:257:GLU:OE2	1:G:313:GLY:N	1.61	1.31
2:D:760:ARG:CD	2:D:762:MET:CE	2.09	1.30
2:D:760:ARG:CD	2:D:762:MET:HE2	1.63	1.28
1:G:255:GLY:O	1:G:309:ARG:HD3	1.17	1.27
1:E:380:LEU:HD11	1:E:477:GLU:HG2	1.14	1.14
2:D:760:ARG:HH11	2:D:762:MET:HE3	1.02	1.10
2:H:561:LEU:HD13	2:H:581:GLU:HG2	1.32	1.10
1:A:270:LYS:NZ	1:A:294:ASP:OD2	1.84	1.09
1:C:250:VAL:HG22	1:C:256:ARG:O	1.49	1.09
1:E:380:LEU:CD1	1:E:477:GLU:HG2	1.84	1.08
1:A:417:LEU:HB3	1:A:421:ALA:HB2	1.25	1.08
2:D:538:LYS:HG3	2:D:543:GLU:HB3	1.36	1.07
1:G:257:GLU:OE2	1:G:313:GLY:CA	2.02	1.07
1:A:471:HIS:CE1	1:A:475:LEU:HD21	1.88	1.06
1:G:255:GLY:O	1:G:309:ARG:CD	2.02	1.06
1:A:55:LEU:HD11	1:A:72:ASP:OD2	1.54	1.06
2:B:463:SER:O	2:B:467:VAL:HG23	1.55	1.05
1:A:482:LEU:HD23	1:A:485:ILE:HD11	1.38	1.04
1:E:381:GLU:HG2	1:E:424:LEU:HD23	1.39	1.03
2:D:760:ARG:NH1	2:D:762:MET:CE	2.23	1.02
2:D:760:ARG:NH1	2:D:762:MET:HE3	1.74	1.02
2:B:572:ALA:HB1	2:B:573:PRO:HD2	1.38	1.02
1:E:417:LEU:O	1:E:417:LEU:HD23	1.61	1.00
1:A:108:ASN:ND2	2:D:427:SER:O	1.95	0.99
2:D:760:ARG:CD	2:D:762:MET:HE3	1.91	0.98
2:D:760:ARG:HH11	2:D:762:MET:CE	1.75	0.98
2:F:659:LEU:H	2:F:659:LEU:HD12	1.30	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:480:ARG:NH2	2:H:523:GLU:OE2	1.97	0.96
1:A:471:HIS:CD2	1:A:475:LEU:HD11	2.00	0.95
2:B:463:SER:HB3	2:B:466:GLU:HB2	1.49	0.94
1:E:380:LEU:HD11	1:E:477:GLU:CG	1.96	0.92
2:H:509:LEU:HD11	3:L:47:ILE:HD11	1.49	0.92
2:H:561:LEU:HB2	2:H:581:GLU:HG3	1.49	0.92
2:B:565:THR:HG22	2:B:576:ALA:HB2	1.47	0.92
1:C:307:VAL:HG12	1:C:308:LYS:O	1.68	0.91
2:D:538:LYS:CG	2:D:543:GLU:HB3	1.99	0.91
1:E:381:GLU:HG3	1:E:478:TYR:HE2	1.33	0.90
1:C:72:ASP:O	1:C:76:LYS:HG3	1.71	0.90
1:A:471:HIS:NE2	1:A:475:LEU:HD11	1.87	0.89
1:A:25:ALA:O	1:A:29:ILE:HG13	1.74	0.88
1:G:91:ARG:HG3	1:G:91:ARG:HH21	1.38	0.87
2:F:699:GLY:C	2:F:700:LEU:HD12	1.95	0.87
1:G:257:GLU:OE2	1:G:313:GLY:HA3	1.74	0.87
1:A:26:MET:SD	1:A:176:VAL:HG21	2.15	0.87
2:D:449:LYS:HD2	2:D:461:MET:HE2	1.57	0.87
2:B:474:LEU:HD21	2:B:514:PHE:CE1	2.10	0.87
1:C:30:VAL:HG13	1:C:34:LEU:HD12	1.56	0.86
2:D:494:ILE:CG2	2:D:530:ALA:HB2	2.04	0.86
2:D:493:ILE:HG13	2:D:527:VAL:HA	1.56	0.86
2:H:509:LEU:CD1	3:L:47:ILE:HD11	2.05	0.86
2:F:596:ARG:HH11	2:F:597:MET:HE2	1.38	0.86
1:G:86:TYR:O	1:G:90:VAL:HG23	1.75	0.86
2:F:612:GLN:O	2:F:698:ARG:NH1	2.08	0.85
2:B:559:ILE:O	2:B:709:ARG:NH2	2.10	0.85
1:E:381:GLU:HG2	1:E:424:LEU:CD2	2.06	0.84
1:A:417:LEU:HB3	1:A:421:ALA:CB	2.06	0.84
1:A:69:VAL:O	1:A:73:VAL:HG23	1.76	0.84
2:B:611:TYR:O	2:B:698:ARG:CD	2.25	0.84
1:G:99:ARG:NH1	1:G:100:TYR:OH	2.11	0.84
1:A:186:ASN:O	1:A:190:VAL:HG23	1.77	0.84
2:B:408:ALA:HB2	2:B:444:LEU:HD13	1.58	0.83
2:H:495:ILE:O	2:H:495:ILE:HG22	1.77	0.83
1:A:99:ARG:HA	1:A:218:PRO:HG3	1.60	0.83
3:K:37:LEU:O	3:K:37:LEU:HD12	1.77	0.82
1:A:70:VAL:O	1:A:74:ILE:HG13	1.78	0.82
1:A:324:THR:HG22	1:A:325:GLN:N	1.96	0.81
2:F:702:GLU:HG2	2:F:703:GLU:H	1.45	0.81
3:I:30:LYS:NZ	3:I:33:GLN:OE1	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:504:SER:O	2:D:508:THR:HG23	1.80	0.80
2:B:474:LEU:HD21	2:B:514:PHE:HE1	1.45	0.80
2:D:529:ILE:O	2:D:762:MET:HB3	1.81	0.80
2:F:457:ARG:HH21	2:F:457:ARG:HG3	1.46	0.80
2:B:468:ALA:O	2:B:471:ILE:HG22	1.81	0.79
2:D:493:ILE:C	2:D:494:ILE:HD13	2.02	0.79
2:D:760:ARG:NH1	2:D:762:MET:HE1	1.95	0.79
2:F:656:GLU:CB	2:F:657:GLN:HA	2.10	0.79
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.47	0.79
1:E:324:THR:HG22	1:E:325:GLN:N	1.98	0.79
1:E:471:HIS:O	1:E:475:LEU:HD13	1.82	0.79
2:B:714:GLN:CG	2:B:715:PRO:HD2	2.13	0.79
2:B:611:TYR:O	2:B:698:ARG:HD3	1.82	0.78
2:F:528:TYR:CE1	2:F:764:ARG:HB2	2.18	0.78
2:D:760:ARG:CZ	2:D:762:MET:CE	2.61	0.78
1:G:257:GLU:O	1:G:307:VAL:HB	1.83	0.78
1:C:317:LEU:O	1:C:317:LEU:HD12	1.83	0.78
1:A:176:VAL:HG13	1:A:177:GLY:N	1.99	0.78
2:B:610:ILE:HG22	2:B:690:ILE:HG23	1.65	0.78
1:C:81:GLY:HA3	3:K:58:ASP:O	1.84	0.78
2:D:479:GLY:HA2	3:K:33:GLN:NE2	1.97	0.77
3:J:61:GLU:HG2	3:J:61:GLU:O	1.84	0.77
2:B:708:GLU:HB2	2:B:713:ARG:HG2	1.64	0.77
2:D:760:ARG:CZ	2:D:762:MET:HE1	2.14	0.77
1:E:79:PRO:HB2	1:G:121:ARG:HB3	1.65	0.77
1:C:74:ILE:O	1:C:79:PRO:HB3	1.85	0.77
2:F:493:ILE:HD11	2:F:527:VAL:HG22	1.65	0.77
2:D:493:ILE:HD11	2:D:527:VAL:HB	1.66	0.77
2:B:697:LEU:HD11	2:B:719:PHE:CG	2.20	0.77
1:C:264:ILE:HB	1:C:265:PRO:HD2	1.67	0.77
2:B:694:GLY:C	2:B:698:ARG:NH1	2.38	0.76
2:B:564:ALA:HB2	2:B:709:ARG:HA	1.67	0.76
2:H:561:LEU:HB2	2:H:581:GLU:CG	2.15	0.76
2:F:699:GLY:O	2:F:700:LEU:HD12	1.85	0.76
1:C:80:HIS:O	3:K:57:ASP:HB2	1.85	0.76
1:A:55:LEU:HD21	1:A:72:ASP:OD2	1.86	0.75
1:C:76:LYS:HE2	1:C:153:GLU:OE2	1.86	0.75
2:B:488:LEU:HD23	2:B:490:TYR:H	1.50	0.75
1:A:38:ARG:NH1	1:A:158:VAL:HG21	2.01	0.75
2:F:653:THR:HG22	2:F:654:ASN:O	1.86	0.75
2:B:464:SER:HB3	3:I:43:GLU:HG2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ASP:OD1	1:C:151:GLY:N	2.20	0.75
1:A:324:THR:HG22	1:A:325:GLN:H	1.52	0.74
2:F:657:GLN:O	2:F:657:GLN:HG2	1.87	0.74
2:B:500:ASP:OD1	2:B:502:ASP:N	2.19	0.74
1:A:83:SER:OG	3:K:62:GLU:OE1	2.04	0.74
1:A:420:VAL:HG12	1:A:471:HIS:CE1	2.23	0.74
2:B:460:LYS:HE2	3:I:46:ARG:HD2	1.68	0.74
1:E:381:GLU:CG	1:E:424:LEU:HD23	2.18	0.73
1:G:74:ILE:HA	1:G:78:HIS:O	1.89	0.73
2:F:457:ARG:NH2	2:F:457:ARG:HG3	2.03	0.73
2:H:561:LEU:CD1	2:H:581:GLU:HG2	2.16	0.73
1:E:381:GLU:HG3	1:E:478:TYR:CE2	2.20	0.73
3:K:27:PHE:CE2	3:K:33:GLN:HG3	2.24	0.73
1:G:290:SER:HB3	1:G:308:LYS:HB3	1.70	0.72
1:E:121:ARG:HB3	1:G:79:PRO:HB2	1.71	0.72
1:A:471:HIS:NE2	1:A:475:LEU:HD21	2.05	0.72
2:B:611:TYR:O	2:B:698:ARG:HD2	1.89	0.72
1:A:66:SER:O	1:A:70:VAL:HG23	1.90	0.72
1:C:245:ARG:NH1	1:C:245:ARG:HG3	2.02	0.72
2:D:760:ARG:NE	2:D:762:MET:CE	2.53	0.71
2:F:559:ILE:HG22	2:F:730:SER:HB2	1.72	0.71
1:C:119:ALA:CB	1:C:121:ARG:HG2	2.20	0.71
1:C:293:ARG:NH1	1:C:295:GLU:OE2	2.21	0.71
2:F:659:LEU:N	2:F:659:LEU:HD12	2.04	0.71
1:G:31:GLY:O	1:G:34:LEU:O	2.09	0.71
2:B:719:PHE:CE2	2:B:723:LEU:HD22	2.25	0.71
1:A:259:ILE:HD13	1:A:317:LEU:CD1	2.21	0.71
2:F:596:ARG:HH11	2:F:597:MET:CE	2.04	0.71
2:B:488:LEU:HD23	2:B:490:TYR:N	2.06	0.71
2:D:529:ILE:HG13	2:D:765:VAL:CG1	2.20	0.70
2:F:494:ILE:HA	2:F:528:TYR:O	1.92	0.70
2:H:495:ILE:HG22	2:H:497:THR:HG22	1.72	0.70
3:K:62:GLU:HA	3:K:62:GLU:OE2	1.91	0.70
2:F:438:ARG:HH22	1:G:299:ASP:HB2	1.56	0.70
2:B:408:ALA:CB	2:B:444:LEU:HD13	2.21	0.70
2:H:419:GLU:OE1	2:H:760:ARG:NH1	2.23	0.70
2:F:529:ILE:O	2:F:762:MET:HB2	1.91	0.70
1:C:197:TYR:OH	1:C:201:GLU:OE2	2.04	0.69
2:B:548:ASP:OD1	2:B:550:GLU:HB3	1.91	0.69
1:C:250:VAL:HG22	1:C:256:ARG:C	2.12	0.69
1:A:212:ILE:HD11	1:A:347:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:ARG:HD2	1:C:158:VAL:HG11	1.74	0.69
2:D:760:ARG:HD2	2:D:762:MET:HE3	1.70	0.69
2:B:712:ARG:HD3	2:B:729:GLU:OE1	1.93	0.69
1:G:120:MET:HG2	1:G:120:MET:O	1.91	0.69
2:F:591:GLN:O	2:F:594:ILE:HG12	1.92	0.69
1:A:55:LEU:CD1	1:A:72:ASP:OD2	2.37	0.69
2:D:403:LEU:N	2:D:404:PRO:CD	2.56	0.69
2:B:537:VAL:HG12	2:B:736:ILE:HG22	1.75	0.69
1:A:39:ASP:O	1:A:165:ASN:ND2	2.21	0.69
1:E:471:HIS:HD2	1:E:475:LEU:HD13	1.59	0.68
2:F:596:ARG:NH1	2:F:597:MET:CE	2.57	0.68
2:F:454:GLU:HG3	2:H:451:LEU:HG	1.75	0.68
1:A:249:GLU:OE2	1:A:260:ILE:HD12	1.94	0.68
2:B:539:LYS:HB2	2:B:734:LEU:HB3	1.75	0.68
2:F:616:THR:HG22	2:F:618:ALA:H	1.59	0.68
1:C:246:ALA:HA	1:C:261:VAL:HA	1.75	0.68
2:B:488:LEU:HD21	2:B:490:TYR:O	1.95	0.67
1:A:99:ARG:HH12	1:A:515:ASP:HB3	1.59	0.67
1:A:81:GLY:O	3:K:61:GLU:HB2	1.93	0.67
1:A:259:ILE:HG22	1:A:260:ILE:N	2.10	0.67
1:E:469:LEU:O	1:E:469:LEU:HD13	1.93	0.67
2:B:714:GLN:HG2	2:B:715:PRO:HD2	1.75	0.67
2:H:461:MET:SD	3:L:45:LYS:O	2.53	0.67
1:C:249:GLU:O	1:C:249:GLU:HG3	1.94	0.67
1:A:398:ARG:NH2	1:C:391:ASP:OD2	2.28	0.67
1:G:416:GLN:HG2	1:G:416:GLN:O	1.94	0.67
1:A:478:TYR:CE2	1:A:482:LEU:CD1	2.78	0.67
2:D:494:ILE:HD13	2:D:494:ILE:N	2.10	0.67
2:B:564:ALA:CB	2:B:709:ARG:HA	2.25	0.67
2:B:422:LEU:HD13	2:B:510:LEU:HD22	1.75	0.66
2:F:569:ASN:ND2	2:F:570:ALA:HB2	2.10	0.66
2:H:459:ASP:OD1	3:L:48:PRO:HA	1.96	0.66
2:D:419:GLU:HB3	2:D:492:SER:HB2	1.76	0.66
1:A:143:VAL:HG21	1:A:158:VAL:HB	1.76	0.66
2:F:705:ALA:HB3	2:F:716:VAL:O	1.94	0.66
2:D:760:ARG:HD3	2:D:762:MET:HE2	0.69	0.66
2:B:694:GLY:HA3	2:B:698:ARG:HH12	1.60	0.66
1:C:119:ALA:HB1	1:C:121:ARG:HG2	1.76	0.66
1:A:259:ILE:O	1:A:260:ILE:HG13	1.96	0.66
1:E:473:LYS:O	1:E:476:ASP:HB2	1.95	0.66
2:H:494:ILE:HA	2:H:528:TYR:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:505:HIS:O	2:D:509:LEU:HG	1.96	0.66
1:A:86:TYR:O	1:A:90:VAL:HG23	1.95	0.66
1:C:390:ILE:O	1:C:394:ILE:HG13	1.95	0.66
1:G:419:ASN:O	1:G:420:VAL:HG22	1.96	0.66
2:B:572:ALA:HB1	2:B:573:PRO:CD	2.20	0.65
2:H:528:TYR:HB3	2:H:762:MET:HE3	1.77	0.65
2:D:529:ILE:HG13	2:D:765:VAL:HG12	1.77	0.65
2:B:425:GLY:N	2:B:446:LEU:O	2.29	0.65
1:C:250:VAL:HG23	1:C:257:GLU:HG2	1.77	0.65
2:B:708:GLU:CB	2:B:713:ARG:HG2	2.26	0.65
1:A:200:ASP:O	1:A:203:ILE:HB	1.96	0.65
2:F:656:GLU:HB3	2:F:657:GLN:HA	1.79	0.65
1:E:469:LEU:HD13	1:E:469:LEU:C	2.17	0.65
1:C:82:ASP:OD2	3:K:60:SER:HB3	1.96	0.65
2:B:634:VAL:O	2:B:638:ASN:ND2	2.30	0.65
1:E:324:THR:HG22	1:E:325:GLN:H	1.61	0.65
1:E:74:ILE:HA	1:E:78:HIS:O	1.97	0.64
3:L:7:VAL:HG21	3:L:18:TRP:HE3	1.62	0.64
1:C:250:VAL:CG2	1:C:256:ARG:O	2.37	0.64
1:A:324:THR:CG2	1:A:325:GLN:H	2.09	0.64
1:E:273:LEU:HD11	1:E:324:THR:HG22	1.80	0.64
1:E:37:VAL:HA	1:E:166:LEU:HD22	1.79	0.64
1:C:265:PRO:HG2	1:C:268:VAL:HG21	1.78	0.64
2:B:488:LEU:CD2	2:B:490:TYR:H	2.11	0.64
2:B:714:GLN:HG2	2:B:715:PRO:CD	2.26	0.64
2:F:616:THR:H	2:F:619:ASP:HB2	1.63	0.64
1:G:259:ILE:HB	1:G:305:ILE:HB	1.79	0.64
1:A:482:LEU:CD2	1:A:485:ILE:HD11	2.21	0.64
1:E:324:THR:CG2	1:E:325:GLN:N	2.61	0.64
1:A:74:ILE:HA	1:A:78:HIS:O	1.98	0.64
1:C:386:ALA:O	1:C:390:ILE:HG13	1.98	0.64
1:A:201:GLU:O	1:A:202:ASP:HB2	1.98	0.64
2:H:480:ARG:CZ	3:L:25:ARG:HD2	2.28	0.63
2:B:718:SER:OG	2:B:719:PHE:N	2.29	0.63
1:A:324:THR:CG2	1:A:325:GLN:N	2.61	0.63
1:A:65:LYS:NZ	1:A:122:TYR:O	2.29	0.63
2:B:408:ALA:CA	2:B:444:LEU:HD13	2.29	0.63
2:F:596:ARG:NH1	2:F:597:MET:HE2	2.11	0.63
1:G:121:ARG:NH2	1:G:122:TYR:CZ	2.66	0.63
1:E:191:ILE:HG21	1:E:510:ARG:HB2	1.79	0.63
1:A:420:VAL:HG12	1:A:471:HIS:NE2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:GLU:HA	1:E:470:GLU:OE1	1.98	0.63
2:B:502:ASP:O	2:B:506:ILE:HD12	1.99	0.63
3:L:7:VAL:HG21	3:L:18:TRP:CE3	2.32	0.63
2:F:616:THR:HG22	2:F:617:GLU:N	2.13	0.63
1:A:478:TYR:CE2	1:A:482:LEU:HD11	2.34	0.63
2:D:493:ILE:HD11	2:D:527:VAL:CB	2.28	0.63
2:F:603:LYS:HG3	2:F:604:ALA:H	1.63	0.62
2:F:603:LYS:HG3	2:F:604:ALA:N	2.14	0.62
1:A:215:PRO:HG2	1:A:223:ILE:CD1	2.29	0.62
1:A:83:SER:O	1:A:87:ASP:HB2	2.00	0.62
1:A:242:ILE:HD11	1:A:330:PHE:HB2	1.80	0.62
1:G:91:ARG:HG3	1:G:91:ARG:NH2	2.08	0.62
2:D:494:ILE:HA	2:D:528:TYR:O	1.99	0.62
1:A:273:LEU:HD21	1:A:326:LEU:HD21	1.81	0.62
2:H:495:ILE:HG21	2:H:507:ARG:HG3	1.81	0.62
2:F:705:ALA:HB3	2:F:716:VAL:HG23	1.81	0.62
2:F:680:GLU:O	2:F:684:GLY:N	2.33	0.62
1:E:273:LEU:HD11	1:E:324:THR:CG2	2.30	0.62
1:E:475:LEU:N	1:E:475:LEU:HD12	2.15	0.62
1:E:380:LEU:HD22	1:E:474:LEU:HD11	1.82	0.62
2:H:509:LEU:HD11	3:L:47:ILE:CD1	2.28	0.62
1:A:395:GLU:O	1:A:398:ARG:HB3	1.99	0.62
2:H:523:GLU:O	2:H:525:GLY:N	2.32	0.62
2:B:564:ALA:HB2	2:B:709:ARG:HG3	1.82	0.61
2:B:568:THR:O	2:B:705:ALA:HB2	2.00	0.61
2:F:421:TYR:HB2	2:F:443:ILE:HD13	1.82	0.61
1:C:312:VAL:O	1:C:316:VAL:HG23	2.00	0.61
1:A:33:ALA:O	1:A:34:LEU:HD23	2.01	0.61
2:D:478:ILE:HD13	3:K:37:LEU:CD2	2.30	0.61
1:G:191:ILE:HG21	1:G:510:ARG:HB2	1.82	0.61
2:H:538:LYS:HG2	2:H:543:GLU:HA	1.83	0.61
2:F:656:GLU:CG	2:F:657:GLN:HA	2.29	0.61
1:A:259:ILE:HD13	1:A:317:LEU:HD12	1.82	0.61
2:D:512:THR:HG21	2:D:777:PHE:HD2	1.65	0.61
1:A:280:LEU:HB3	1:A:286:VAL:HG12	1.81	0.61
1:E:324:THR:CG2	1:E:325:GLN:H	2.13	0.61
2:H:419:GLU:CD	2:H:760:ARG:HH12	2.04	0.61
2:B:464:SER:HB3	3:I:43:GLU:CG	2.30	0.61
1:A:189:GLU:HB3	1:A:212:ILE:HG22	1.82	0.61
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.64	0.61
1:G:67:ALA:HB2	1:G:120:MET:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:494:ILE:HG22	2:D:530:ALA:HB2	1.83	0.61
2:F:702:GLU:HG2	2:F:703:GLU:N	2.15	0.61
2:B:714:GLN:HG3	2:B:715:PRO:HD2	1.82	0.61
2:B:475:GLY:HA3	2:B:489:ARG:HG3	1.81	0.61
2:H:761:ARG:NH1	2:H:762:MET:O	2.34	0.61
1:C:121:ARG:HG3	1:C:122:TYR:CE1	2.36	0.61
1:A:416:GLN:C	1:A:417:LEU:HD12	2.21	0.60
3:K:39:GLU:HB3	3:K:44:GLU:HB2	1.83	0.60
1:E:65:LYS:NZ	1:E:122:TYR:O	2.31	0.60
1:C:427:ALA:HB1	1:C:482:LEU:HD13	1.82	0.60
2:B:594:ILE:HG22	2:B:603:LYS:HG3	1.82	0.60
2:F:607:LYS:O	2:F:610:ILE:HG13	2.01	0.60
2:F:656:GLU:HG2	2:F:657:GLN:HA	1.83	0.60
1:A:21:TYR:O	1:A:24:TYR:HB3	2.01	0.60
1:E:444:ARG:O	1:E:445:ASP:HB2	2.01	0.60
1:C:358:ARG:NH2	1:C:505:GLU:OE1	2.34	0.60
2:B:611:TYR:CE1	2:B:697:LEU:HD22	2.36	0.60
1:E:471:HIS:CD2	1:E:475:LEU:HD13	2.37	0.60
1:A:244:ALA:HB2	1:A:265:PRO:HD3	1.82	0.60
1:C:381:GLU:O	1:C:385:VAL:HG23	2.01	0.60
1:G:75:GLY:O	1:G:149:TYR:OH	2.15	0.60
1:E:417:LEU:O	1:E:417:LEU:CD2	2.44	0.60
1:E:390:ILE:HG21	1:G:398:ARG:HH12	1.66	0.60
2:B:564:ALA:HB2	2:B:709:ARG:CG	2.32	0.59
2:B:696:LYS:O	2:B:700:LEU:HD22	2.02	0.59
1:C:305:ILE:O	1:C:305:ILE:HG22	2.01	0.59
2:B:694:GLY:CA	2:B:698:ARG:HH12	2.14	0.59
1:C:230:GLU:HG2	1:C:234:ARG:HH12	1.68	0.59
1:G:255:GLY:HA3	1:G:309:ARG:NH1	2.17	0.59
2:F:659:LEU:H	2:F:659:LEU:CD1	2.05	0.59
1:E:273:LEU:CD1	1:E:324:THR:CG2	2.80	0.59
1:E:260:ILE:HD13	1:E:302:ARG:NH1	2.18	0.59
1:E:381:GLU:OE2	1:E:478:TYR:OH	2.12	0.59
2:D:479:GLY:HA2	3:K:33:GLN:HE22	1.67	0.59
1:C:254:THR:HG22	1:C:254:THR:O	2.02	0.59
2:D:494:ILE:HG21	2:D:530:ALA:HB2	1.84	0.59
1:E:393:ILE:HD13	1:E:458:ILE:HD11	1.84	0.59
2:B:494:ILE:HA	2:B:528:TYR:O	2.03	0.59
1:A:358:ARG:NH2	1:A:505:GLU:OE1	2.36	0.59
3:K:37:LEU:C	3:K:37:LEU:HD12	2.23	0.59
1:G:358:ARG:NH2	1:G:505:GLU:OE1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:ALA:O	1:C:426:ARG:HB2	2.03	0.59
3:I:16:VAL:HG11	3:I:28:CYS:HA	1.84	0.59
2:B:714:GLN:HG2	2:B:715:PRO:N	2.18	0.58
2:B:602:PRO:HD2	2:B:605:MET:CE	2.32	0.58
2:B:463:SER:CB	2:B:466:GLU:HB2	2.29	0.58
2:B:694:GLY:CA	2:B:698:ARG:NH1	2.66	0.58
1:A:259:ILE:HD13	1:A:317:LEU:HD13	1.85	0.58
1:G:244:ALA:HB2	1:G:265:PRO:HD3	1.84	0.58
2:B:409:ASP:O	2:B:442:ALA:HB1	2.04	0.58
1:G:209:MET:HE1	1:G:230:GLU:HA	1.84	0.58
1:C:32:ARG:O	1:C:32:ARG:HG2	2.02	0.58
1:C:245:ARG:HG2	1:C:245:ARG:O	2.02	0.58
2:D:419:GLU:CB	2:D:492:SER:HB2	2.33	0.58
1:A:203:ILE:O	1:A:348:LYS:NZ	2.36	0.58
1:A:82:ASP:C	1:A:84:ALA:H	2.07	0.58
1:E:444:ARG:HG3	1:E:444:ARG:O	2.03	0.58
1:A:422:ALA:O	1:A:426:ARG:HB2	2.03	0.58
1:C:324:THR:HB	1:C:326:LEU:HD13	1.85	0.58
1:E:462:ARG:NH2	1:E:464:GLN:OE1	2.36	0.58
1:C:37:VAL:HA	1:C:166:LEU:HD22	1.85	0.58
3:K:42:ALA:HB3	3:K:44:GLU:HG2	1.86	0.58
1:C:391:ASP:N	1:C:392:PRO:CD	2.66	0.58
2:B:517:GLN:OE1	3:I:33:GLN:NE2	2.37	0.58
2:F:751:TRP:HA	2:F:755:MET:HB2	1.86	0.58
2:B:474:LEU:HD23	2:B:518:MET:SD	2.44	0.57
2:D:515:TYR:HB2	2:D:770:ALA:HB1	1.86	0.57
2:D:420:LEU:HB3	2:D:493:ILE:HG22	1.86	0.57
2:H:751:TRP:HA	2:H:755:MET:HB2	1.85	0.57
1:C:74:ILE:HA	1:C:78:HIS:O	2.04	0.57
2:D:479:GLY:CA	3:K:33:GLN:NE2	2.67	0.57
2:B:464:SER:HB2	3:I:41:ALA:O	2.04	0.57
2:B:500:ASP:OD1	2:B:501:VAL:N	2.38	0.57
1:A:176:VAL:CG1	1:A:177:GLY:N	2.67	0.57
1:A:295:GLU:OE1	1:A:302:ARG:NH2	2.36	0.57
2:H:448:GLY:O	2:H:449:LYS:HB2	2.04	0.57
1:C:39:ASP:O	1:C:165:ASN:ND2	2.35	0.57
1:G:320:LEU:HB3	1:G:326:LEU:HD12	1.87	0.57
1:A:99:ARG:CA	1:A:218:PRO:HG3	2.33	0.57
2:F:751:TRP:CE2	1:G:298:LYS:NZ	2.73	0.57
2:H:766:THR:O	2:H:769:ASP:HB2	2.03	0.57
2:B:488:LEU:HD23	2:B:489:ARG:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:489:ARG:NH2	2:B:490:TYR:OH	2.38	0.56
2:F:609:LEU:HB3	2:F:690:ILE:HD13	1.87	0.56
1:A:203:ILE:HG23	1:A:204:SER:N	2.20	0.56
1:E:362:VAL:HG13	1:E:365:ARG:HH21	1.69	0.56
1:E:463:LEU:HD12	1:G:461:LEU:HB3	1.85	0.56
1:A:471:HIS:O	1:A:472:GLU:C	2.43	0.56
2:B:488:LEU:HD21	2:B:490:TYR:C	2.25	0.56
2:B:421:TYR:HB2	2:B:443:ILE:HG22	1.87	0.56
2:B:601:TYR:HB3	2:B:605:MET:CE	2.35	0.56
1:C:173:GLY:HA3	1:C:180:THR:H	1.69	0.56
2:H:527:VAL:HB	2:H:765:VAL:CG2	2.35	0.56
1:E:469:LEU:HD11	1:E:473:LYS:HG3	1.88	0.56
1:C:23:ASP:O	1:C:26:MET:HB3	2.05	0.56
1:A:68:ARG:HH12	1:C:76:LYS:CE	2.19	0.56
1:C:149:TYR:CG	1:C:150:ASP:N	2.71	0.56
2:F:512:THR:O	2:F:516:ARG:HG3	2.05	0.56
1:C:162:LYS:HA	1:C:358:ARG:NH1	2.20	0.56
1:E:230:GLU:OE2	1:E:234:ARG:NH1	2.39	0.56
1:E:471:HIS:HD2	1:E:475:LEU:CD1	2.18	0.56
2:B:607:LYS:O	2:B:610:ILE:HG12	2.05	0.56
2:H:463:SER:O	2:H:467:VAL:HG23	2.05	0.56
1:A:164:PRO:O	1:A:166:LEU:N	2.39	0.56
1:C:58:ASP:OD2	1:C:61:LYS:NZ	2.39	0.56
2:F:596:ARG:NH1	2:F:597:MET:HE1	2.20	0.55
2:B:488:LEU:HD23	2:B:488:LEU:C	2.27	0.55
1:E:270:LYS:NZ	1:E:294:ASP:OD2	2.39	0.55
1:G:82:ASP:C	1:G:84:ALA:H	2.09	0.55
2:B:421:TYR:CZ	2:B:494:ILE:HD12	2.41	0.55
1:G:195:LEU:HA	1:G:198:ILE:HG22	1.88	0.55
1:A:407:LYS:HD2	1:A:452:GLU:HG3	1.88	0.55
2:F:480:ARG:NH2	2:F:523:GLU:OE2	2.29	0.55
3:L:16:VAL:HG11	3:L:27:PHE:O	2.06	0.55
2:F:406:LYS:O	2:F:406:LYS:HG2	2.07	0.55
1:C:30:VAL:HG11	1:C:342:PRO:HG3	1.87	0.55
1:A:164:PRO:HB2	1:A:168:VAL:HG23	1.88	0.55
2:B:522:VAL:HG13	2:B:765:VAL:HG23	1.88	0.55
2:F:652:HIS:HB3	2:F:661:GLU:HB3	1.89	0.55
2:B:715:PRO:C	2:B:716:VAL:HG13	2.27	0.55
1:A:108:ASN:HB2	2:D:431:SER:HB3	1.89	0.55
1:A:469:LEU:HD13	1:C:401:PRO:HB3	1.88	0.55
1:A:22:LEU:O	1:A:26:MET:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:36:ASP:OD1	3:K:45:LYS:CE	2.55	0.55
2:D:460:LYS:HE3	2:D:502:ASP:CG	2.26	0.55
2:H:452:ASN:C	2:H:453:VAL:HG23	2.27	0.55
2:B:498:ASP:O	2:B:499:ALA:HB3	2.06	0.55
1:C:209:MET:HE1	1:C:230:GLU:HA	1.88	0.54
3:L:9:CYS:SG	3:L:10:PRO:HD2	2.47	0.54
3:K:31:ARG:O	3:K:35:ILE:HG13	2.06	0.54
2:B:408:ALA:CA	2:B:444:LEU:CD1	2.85	0.54
1:C:264:ILE:HG12	1:C:301:MET:CE	2.38	0.54
1:A:365:ARG:NH2	1:A:505:GLU:OE2	2.33	0.54
1:C:335:VAL:HG22	1:C:344:ILE:HG12	1.90	0.54
1:C:199:ASP:OD1	1:C:503:ARG:NH1	2.41	0.54
1:A:68:ARG:HH12	1:C:76:LYS:HE3	1.72	0.54
1:A:81:GLY:HA3	1:C:82:ASP:OD2	2.07	0.54
2:F:471:ILE:HD11	2:F:478:ILE:HG22	1.89	0.54
2:B:697:LEU:HD11	2:B:719:PHE:CD1	2.43	0.54
2:B:701:LEU:HD23	2:B:702:GLU:N	2.22	0.54
2:B:408:ALA:N	2:B:444:LEU:CD1	2.71	0.54
2:B:452:ASN:O	2:B:458:TYR:N	2.41	0.54
2:B:567:HIS:O	2:B:705:ALA:HB1	2.08	0.54
2:H:531:GLN:NE2	2:H:763:LEU:HB2	2.23	0.54
1:C:273:LEU:O	1:C:277:ILE:HG13	2.08	0.54
1:A:209:MET:HE1	1:A:230:GLU:HA	1.89	0.54
3:L:17:VAL:HG11	3:L:21:ILE:HG21	1.90	0.54
1:E:517:ARG:HD3	1:E:519:THR:O	2.07	0.54
1:C:119:ALA:HB3	1:C:121:ARG:HG2	1.89	0.54
2:F:667:ARG:HG2	2:F:672:ASP:HA	1.90	0.54
1:C:301:MET:O	1:C:302:ARG:HG3	2.08	0.53
2:F:745:MET:HB2	2:F:749:GLN:HB2	1.90	0.53
1:G:247:GLU:HA	1:G:247:GLU:OE1	2.08	0.53
2:B:572:ALA:CB	2:B:573:PRO:HD2	2.23	0.53
1:E:280:LEU:HB3	1:E:286:VAL:HG12	1.90	0.53
1:C:424:LEU:HD12	1:C:425:GLU:N	2.24	0.53
2:H:580:LEU:O	2:H:583:LEU:HB3	2.07	0.53
1:A:293:ARG:NH1	1:A:295:GLU:OE2	2.41	0.53
1:C:82:ASP:N	1:C:82:ASP:OD1	2.39	0.53
2:F:705:ALA:CB	2:F:716:VAL:HG23	2.38	0.53
2:D:511:LEU:O	2:D:515:TYR:N	2.36	0.53
2:H:423:VAL:HA	2:H:496:MET:O	2.09	0.53
1:A:471:HIS:O	1:A:474:LEU:N	2.42	0.53
2:D:461:MET:SD	3:K:43:GLU:HB3	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:548:ASP:OD1	2:D:549:ASP:N	2.42	0.53
2:B:702:GLU:HA	2:B:702:GLU:OE1	2.09	0.53
1:G:221:ALA:H	1:G:519:THR:HG22	1.73	0.53
2:B:565:THR:HG22	2:B:576:ALA:CB	2.30	0.53
1:E:80:HIS:ND1	3:J:57:ASP:HB3	2.23	0.53
2:F:428:ALA:HB2	2:F:742:LEU:HB3	1.90	0.53
2:F:409:ASP:OD1	2:F:490:TYR:OH	2.27	0.53
2:D:493:ILE:HD11	2:D:527:VAL:CG1	2.39	0.53
2:D:480:ARG:HD2	3:K:25:ARG:HB2	1.89	0.53
2:F:702:GLU:CG	2:F:703:GLU:H	2.15	0.52
3:K:27:PHE:CD2	3:K:33:GLN:HG3	2.45	0.52
2:B:527:VAL:O	2:B:765:VAL:HG22	2.08	0.52
1:A:155:ILE:HD12	1:A:156:PRO:HD2	1.92	0.52
1:C:182:ILE:HG12	1:C:334:MET:HG2	1.91	0.52
1:A:414:PRO:O	1:A:415:TRP:HD1	1.92	0.52
1:A:517:ARG:CG	1:A:517:ARG:HH11	2.19	0.52
2:B:701:LEU:HD13	2:B:718:SER:HA	1.91	0.52
1:G:70:VAL:O	1:G:74:ILE:HG13	2.09	0.52
1:A:129:LYS:HB3	1:A:513:PHE:CE1	2.45	0.52
2:B:431:SER:HB3	2:B:750:LEU:HD22	1.90	0.52
2:D:449:LYS:HG2	2:D:450:ILE:N	2.23	0.52
3:I:16:VAL:HG11	3:I:28:CYS:CA	2.39	0.52
1:A:342:PRO:C	1:A:343:LYS:HG2	2.30	0.52
1:E:380:LEU:HD22	1:E:474:LEU:CD1	2.39	0.52
2:B:719:PHE:HE2	2:B:723:LEU:HD22	1.72	0.52
1:G:99:ARG:NH1	1:G:100:TYR:CZ	2.77	0.52
2:B:715:PRO:O	2:B:716:VAL:CG1	2.57	0.52
1:C:270:LYS:NZ	1:C:294:ASP:OD2	2.43	0.52
2:F:716:VAL:HG21	2:F:722:ALA:HB2	1.91	0.52
1:G:89:ILE:HG21	1:G:125:ILE:HD13	1.91	0.52
1:E:220:ALA:HB1	1:E:263:GLU:OE1	2.10	0.52
1:A:417:LEU:HD23	1:A:421:ALA:CB	2.40	0.52
1:G:438:GLU:O	1:G:440:GLU:N	2.41	0.52
2:D:459:ASP:N	3:K:46:ARG:HD3	2.25	0.52
2:F:529:ILE:HG12	2:F:765:VAL:HG13	1.91	0.52
2:D:777:PHE:O	2:D:781:MET:N	2.43	0.52
2:D:593:MET:HE2	2:D:596:ARG:HH22	1.74	0.52
2:H:490:TYR:HB2	2:H:493:ILE:HD11	1.92	0.52
2:F:528:TYR:OH	2:F:764:ARG:CZ	2.57	0.52
2:H:495:ILE:CG2	2:H:495:ILE:O	2.47	0.51
1:A:75:GLY:O	1:A:149:TYR:OH	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:TYR:N	1:C:122:TYR:CD1	2.76	0.51
2:F:599:ARG:HG3	2:F:599:ARG:HH11	1.75	0.51
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.73	0.51
2:F:599:ARG:NH1	2:F:599:ARG:HG3	2.25	0.51
1:C:250:VAL:HA	1:C:257:GLU:HA	1.93	0.51
1:A:259:ILE:CG2	1:A:260:ILE:N	2.73	0.51
1:E:70:VAL:O	1:E:74:ILE:HG13	2.10	0.51
1:E:459:LEU:O	1:G:464:GLN:N	2.43	0.51
1:G:37:VAL:HA	1:G:166:LEU:HD22	1.92	0.51
2:B:711:GLU:OE2	2:B:711:GLU:HA	2.10	0.51
1:A:501:VAL:O	1:A:504:GLU:HG2	2.11	0.51
2:H:412:GLU:HG2	2:H:417:LEU:HB2	1.92	0.51
1:G:130:ILE:HD12	1:G:130:ILE:H	1.76	0.51
2:B:766:THR:HB	2:B:768:LYS:HG2	1.93	0.51
1:A:416:GLN:O	1:A:417:LEU:HD12	2.11	0.51
2:H:497:THR:OG1	2:H:498:ASP:N	2.43	0.51
1:E:475:LEU:N	1:E:475:LEU:CD1	2.73	0.51
1:C:70:VAL:O	1:C:71:GLY:C	2.49	0.51
1:E:38:ARG:HE	1:E:158:VAL:HG11	1.75	0.51
1:E:293:ARG:HD2	1:E:295:GLU:OE2	2.11	0.51
1:E:345:MET:HB3	1:E:350:ILE:HG13	1.93	0.51
1:C:85:VAL:HG12	1:C:85:VAL:O	2.09	0.51
3:J:40:TRP:CD2	3:J:45:LYS:HG3	2.46	0.51
1:A:471:HIS:CD2	1:A:475:LEU:CD1	2.86	0.51
1:C:201:GLU:OE1	1:C:202:ASP:N	2.39	0.51
2:B:483:TYR:CD2	2:B:520:GLU:HB2	2.46	0.51
1:G:106:GLN:HB3	1:G:124:GLU:HG3	1.93	0.51
1:G:420:VAL:O	1:G:420:VAL:HG23	2.11	0.51
1:A:354:PHE:O	1:A:357:HIS:HB3	2.11	0.51
3:J:30:LYS:HZ2	3:J:33:GLN:NE2	2.09	0.51
1:C:451:THR:N	1:C:454:GLN:OE1	2.44	0.51
1:G:416:GLN:O	1:G:416:GLN:CG	2.59	0.50
2:B:567:HIS:ND1	2:B:706:PHE:HB3	2.25	0.50
1:C:58:ASP:HA	1:C:132:HIS:CE1	2.46	0.50
2:F:412:GLU:HG2	2:F:417:LEU:HB2	1.92	0.50
1:E:401:PRO:HA	1:G:468:GLY:HA3	1.93	0.50
1:A:165:ASN:H	1:A:168:VAL:CG2	2.25	0.50
1:E:393:ILE:HG23	1:E:410:LEU:HD21	1.92	0.50
3:L:8:ASN:HA	3:L:15:THR:HA	1.93	0.50
2:H:400:LEU:HD23	2:H:404:PRO:HG3	1.94	0.50
1:A:381:GLU:OE2	1:A:433:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:PRO:HA	1:A:448:TYR:O	2.11	0.50
3:K:57:ASP:N	3:K:57:ASP:OD1	2.44	0.50
2:F:701:LEU:HD23	2:F:705:ALA:HB2	1.93	0.50
2:F:702:GLU:CG	2:F:703:GLU:N	2.73	0.50
2:F:601:TYR:HB2	2:F:606:LEU:HD11	1.94	0.50
1:G:91:ARG:CG	1:G:91:ARG:NH2	2.73	0.50
1:A:82:ASP:C	1:A:84:ALA:N	2.65	0.50
2:F:438:ARG:HD2	1:G:302:ARG:HH21	1.77	0.50
3:J:30:LYS:NZ	3:J:33:GLN:NE2	2.60	0.50
1:A:381:GLU:OE1	1:A:433:ARG:NH1	2.42	0.50
2:F:465:GLN:O	2:F:469:THR:OG1	2.15	0.50
1:C:189:GLU:OE1	1:C:517:ARG:NH1	2.45	0.50
1:E:83:SER:HB3	3:J:60:SER:HB2	1.92	0.50
1:A:389:ASN:O	1:A:393:ILE:HG22	2.12	0.50
2:D:754:THR:OG1	2:D:754:THR:O	2.28	0.50
2:F:597:MET:O	2:F:600:ARG:HB3	2.11	0.49
2:F:610:ILE:C	2:F:610:ILE:HD12	2.32	0.49
1:G:83:SER:O	1:G:87:ASP:HB2	2.12	0.49
1:E:176:VAL:HG23	1:E:177:GLY:N	2.26	0.49
1:E:319:ASN:HB3	1:E:323:GLN:NE2	2.28	0.49
1:G:205:ILE:HD12	1:G:234:ARG:HG2	1.94	0.49
1:A:471:HIS:HE2	1:A:475:LEU:HD11	1.70	0.49
2:D:549:ASP:HA	2:D:552:MET:HB3	1.95	0.49
2:B:516:ARG:HH12	3:I:45:LYS:HZ2	1.59	0.49
1:G:90:VAL:HG13	1:G:109:PHE:CD2	2.47	0.49
2:H:423:VAL:HG21	2:H:429:GLY:HA2	1.94	0.49
1:E:41:LEU:HB3	1:E:45:HIS:HB2	1.94	0.49
1:C:260:ILE:HA	1:C:303:ILE:O	2.12	0.49
2:F:497:THR:C	2:F:498:ASP:O	2.49	0.49
1:C:142:THR:HG21	1:C:361:VAL:HG13	1.95	0.49
2:B:446:LEU:HD22	2:B:466:GLU:HG2	1.95	0.49
2:F:696:LYS:O	2:F:700:LEU:HD13	2.13	0.49
2:D:478:ILE:O	2:D:478:ILE:HD12	2.13	0.49
2:D:504:SER:O	2:D:508:THR:CG2	2.59	0.49
1:E:273:LEU:CD1	1:E:324:THR:HG22	2.42	0.49
1:E:471:HIS:CD2	1:E:475:LEU:CD1	2.95	0.49
1:C:58:ASP:HA	1:C:132:HIS:HE1	1.77	0.49
2:F:634:VAL:HG21	2:F:649:PHE:HB3	1.93	0.49
1:A:176:VAL:HG13	1:A:177:GLY:H	1.78	0.49
2:F:694:GLY:O	2:F:698:ARG:HB2	2.12	0.49
1:C:274:ILE:HG23	1:C:292:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:LEU:HD11	1:C:326:LEU:HD12	1.94	0.49
1:A:342:PRO:O	1:A:343:LYS:HG2	2.13	0.49
1:A:480:GLU:O	1:A:484:GLN:HG2	2.12	0.49
1:E:478:TYR:CE1	1:E:482:LEU:HD13	2.47	0.49
2:B:708:GLU:HG3	2:B:708:GLU:O	2.13	0.49
1:C:390:ILE:HD13	1:C:466:LEU:HD22	1.94	0.49
1:G:297:ASP:OD2	1:G:298:LYS:HG2	2.13	0.49
2:B:715:PRO:O	2:B:716:VAL:HG13	2.13	0.49
1:C:69:VAL:O	1:C:70:VAL:C	2.50	0.49
1:E:407:LYS:O	1:E:411:VAL:HG13	2.13	0.49
1:C:270:LYS:HD3	1:C:301:MET:CE	2.42	0.48
3:L:18:TRP:CD1	3:L:18:TRP:C	2.85	0.48
2:B:494:ILE:HG22	2:B:530:ALA:HB2	1.94	0.48
1:C:218:PRO:HA	1:C:518:ARG:HH21	1.78	0.48
2:B:606:LEU:HA	2:B:609:LEU:HB2	1.95	0.48
2:B:480:ARG:HH21	3:I:25:ARG:HG3	1.78	0.48
1:G:389:ASN:O	1:G:393:ILE:HG12	2.12	0.48
1:C:285:ARG:HB3	1:C:285:ARG:HH11	1.77	0.48
1:C:285:ARG:HB3	1:C:285:ARG:NH1	2.28	0.48
3:J:8:ASN:ND2	3:J:13:GLY:O	2.46	0.48
2:B:534:LEU:HD23	2:B:535:TYR:CE2	2.49	0.48
2:B:697:LEU:HD11	2:B:719:PHE:CB	2.44	0.48
1:G:66:SER:O	1:G:70:VAL:HG23	2.14	0.48
1:C:386:ALA:O	1:C:390:ILE:CG1	2.61	0.48
1:G:221:ALA:N	1:G:519:THR:HG22	2.28	0.48
1:A:68:ARG:NH1	1:C:76:LYS:HE3	2.29	0.48
3:K:38:GLY:O	3:K:42:ALA:N	2.43	0.48
2:F:569:ASN:HB2	2:F:704:ASP:O	2.13	0.48
2:F:686:GLU:O	2:F:690:ILE:HG23	2.13	0.48
2:H:527:VAL:HB	2:H:765:VAL:HG22	1.96	0.48
3:J:30:LYS:NZ	3:J:33:GLN:HE21	2.12	0.48
2:F:616:THR:CG2	2:F:617:GLU:N	2.75	0.48
2:B:421:TYR:CE1	2:B:494:ILE:HD12	2.49	0.48
2:B:523:GLU:OE2	3:I:18:TRP:HZ2	1.96	0.48
3:K:36:ASP:O	3:K:40:TRP:HD1	1.97	0.48
1:E:79:PRO:HG2	1:G:121:ARG:HD2	1.95	0.48
2:F:610:ILE:HD11	2:F:611:TYR:CD1	2.48	0.48
2:B:602:PRO:HD2	2:B:605:MET:HE2	1.94	0.48
1:A:266:TYR:O	1:A:267:GLN:HB2	2.12	0.48
3:K:24:PHE:CZ	3:K:30:LYS:HB2	2.48	0.48
1:A:55:LEU:CD2	1:A:72:ASP:OD2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:694:GLY:C	2:B:698:ARG:HH12	2.15	0.48
1:A:38:ARG:HD2	1:A:158:VAL:HG11	1.94	0.48
1:A:393:ILE:HG13	1:A:410:LEU:HD21	1.95	0.48
1:C:111:SER:HB3	1:C:115:ASP:HB2	1.95	0.48
2:B:497:THR:HG21	2:B:503:GLY:O	2.14	0.48
1:G:259:ILE:O	1:G:260:ILE:HG13	2.13	0.48
1:G:121:ARG:NH2	1:G:122:TYR:OH	2.46	0.48
1:A:288:GLY:HA2	1:A:308:LYS:HE2	1.95	0.48
2:B:719:PHE:O	2:B:720:GLU:C	2.52	0.47
2:F:411:GLN:OE1	1:G:302:ARG:NH2	2.47	0.47
2:F:569:ASN:CG	2:F:704:ASP:H	2.17	0.47
1:G:166:LEU:HD11	1:G:182:ILE:HD12	1.96	0.47
2:B:411:GLN:HG2	2:B:439:LYS:HA	1.94	0.47
2:H:548:ASP:OD1	2:H:549:ASP:N	2.47	0.47
2:F:767:VAL:O	2:F:771:ILE:HG13	2.14	0.47
1:G:111:SER:OG	1:G:115:ASP:OD2	2.32	0.47
1:A:417:LEU:N	1:A:417:LEU:HD12	2.30	0.47
1:C:74:ILE:HG23	1:C:79:PRO:HA	1.96	0.47
1:E:408:THR:HA	1:E:411:VAL:HG22	1.96	0.47
1:C:63:TYR:HB3	1:C:124:GLU:HB3	1.96	0.47
2:B:564:ALA:HB2	2:B:709:ARG:CA	2.40	0.47
2:B:460:LYS:CE	3:I:46:ARG:HD2	2.42	0.47
1:E:398:ARG:NH1	1:G:390:ILE:HD12	2.29	0.47
2:B:481:ASP:N	2:B:481:ASP:OD1	2.48	0.47
1:G:275:GLU:O	1:G:275:GLU:HG3	2.14	0.47
2:D:538:LYS:HD3	2:D:540:GLY:HA2	1.95	0.47
1:A:68:ARG:HA	1:C:75:GLY:CA	2.45	0.47
1:E:45:HIS:CD2	1:E:45:HIS:H	2.32	0.47
1:G:113:ASP:OD1	1:G:270:LYS:NZ	2.32	0.47
2:B:749:GLN:O	2:B:753:THR:HG23	2.14	0.47
1:E:402:THR:HG22	1:E:404:ALA:H	1.79	0.47
1:A:260:ILE:HG23	1:A:302:ARG:HG3	1.97	0.47
1:E:182:ILE:HG12	1:E:334:MET:HA	1.97	0.47
1:G:139:GLU:OE2	1:G:140:LYS:HE3	2.15	0.47
1:G:90:VAL:O	1:G:94:GLN:HG3	2.14	0.47
2:B:539:LYS:NZ	2:B:733:GLY:HA3	2.30	0.47
2:F:705:ALA:O	2:F:715:PRO:HA	2.15	0.47
2:B:602:PRO:HD2	2:B:605:MET:HE1	1.96	0.47
1:E:358:ARG:O	1:E:362:VAL:HG23	2.15	0.47
2:H:496:MET:HA	2:H:530:ALA:HB3	1.96	0.47
1:A:181:ASN:ND2	1:A:331:GLY:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:ILE:HG23	1:E:305:ILE:CG2	2.45	0.47
1:C:264:ILE:HB	1:C:265:PRO:CD	2.42	0.47
2:B:488:LEU:CD2	2:B:490:TYR:N	2.72	0.47
2:H:494:ILE:HG12	2:H:528:TYR:HB2	1.95	0.47
1:A:414:PRO:HG2	1:A:414:PRO:O	2.15	0.47
1:C:185:HIS:HA	1:C:216:ASP:H	1.80	0.47
2:F:404:PRO:HG2	2:F:405:GLY:N	2.30	0.47
2:B:697:LEU:O	2:B:697:LEU:HD23	2.15	0.47
1:A:100:TYR:HE1	1:A:515:ASP:OD2	1.98	0.47
2:B:460:LYS:HE2	2:B:461:MET:HE2	1.96	0.47
1:G:55:LEU:HD11	1:G:72:ASP:OD2	2.15	0.47
1:A:124:GLU:C	1:A:125:ILE:HG23	2.34	0.47
2:D:464:SER:HA	2:D:467:VAL:HG12	1.96	0.47
2:H:515:TYR:CD2	2:H:774:ASP:HB2	2.50	0.47
1:C:24:TYR:CE1	1:C:28:VAL:HG23	2.50	0.47
1:E:237:ARG:NE	1:E:333:ASN:OD1	2.44	0.47
2:B:470:LEU:CD1	2:B:474:LEU:HD13	2.45	0.46
2:F:657:GLN:OE1	2:F:657:GLN:N	2.47	0.46
1:A:259:ILE:HB	1:A:305:ILE:HB	1.97	0.46
2:H:407:LEU:HD11	2:H:420:LEU:HD11	1.97	0.46
2:B:516:ARG:NH1	3:I:45:LYS:NZ	2.64	0.46
1:A:401:PRO:HA	1:C:468:GLY:H	1.80	0.46
1:C:129:LYS:HE3	1:C:513:PHE:HE1	1.80	0.46
1:C:301:MET:O	1:C:302:ARG:CG	2.63	0.46
1:G:89:ILE:HD13	1:G:125:ILE:CD1	2.45	0.46
2:F:414:ASP:OD2	2:F:417:LEU:HG	2.15	0.46
1:E:491:ILE:HG22	1:E:497:ARG:HE	1.80	0.46
2:F:595:ASN:O	2:F:598:GLU:HB3	2.15	0.46
1:A:134:LEU:HG	1:A:163:ILE:HD11	1.97	0.46
2:B:445:PRO:O	2:B:446:LEU:HD23	2.15	0.46
1:C:75:GLY:O	1:C:149:TYR:OH	2.30	0.46
1:E:387:LEU:CD2	1:E:471:HIS:HB2	2.46	0.46
2:F:616:THR:HG22	2:F:618:ALA:N	2.29	0.46
1:A:222:ILE:HG22	1:A:223:ILE:N	2.30	0.46
1:E:183:PRO:HD3	1:E:332:ILE:HG23	1.97	0.46
2:F:407:LEU:CD1	2:F:444:LEU:HB2	2.45	0.46
1:A:68:ARG:HA	1:C:75:GLY:HA2	1.96	0.46
2:H:495:ILE:CG2	2:H:497:THR:HG22	2.44	0.46
1:A:165:ASN:N	1:A:168:VAL:HG23	2.30	0.46
1:G:358:ARG:O	1:G:362:VAL:HG22	2.16	0.46
1:E:109:PHE:CE1	1:E:123:THR:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:469:LEU:HB3	1:G:401:PRO:O	2.15	0.46
1:C:136:ALA:HB3	1:C:162:LYS:HE2	1.98	0.46
1:A:63:TYR:HB3	1:A:124:GLU:HB2	1.96	0.46
1:A:401:PRO:HA	1:C:468:GLY:N	2.30	0.46
2:F:457:ARG:CG	2:F:457:ARG:HH21	2.19	0.46
2:D:538:LYS:HG2	2:D:542:GLN:O	2.14	0.46
1:A:388:ALA:HB2	1:A:420:VAL:HG21	1.98	0.46
1:C:38:ARG:HB3	1:C:357:HIS:CD2	2.50	0.46
2:H:527:VAL:O	2:H:765:VAL:HG22	2.16	0.46
2:F:517:GLN:HE21	3:J:37:LEU:HB2	1.81	0.46
2:B:452:ASN:HB3	2:B:460:LYS:HZ2	1.80	0.46
3:L:24:PHE:CZ	3:L:30:LYS:HB2	2.51	0.46
2:H:537:VAL:HA	2:H:735:SER:O	2.15	0.46
2:H:561:LEU:CB	2:H:581:GLU:HG3	2.33	0.46
2:B:611:TYR:HE1	2:B:697:LEU:HD22	1.78	0.46
2:F:528:TYR:CD1	2:F:764:ARG:HB2	2.49	0.46
1:E:36:ASP:OD2	1:E:38:ARG:NH2	2.49	0.46
2:F:737:GLN:HE21	2:F:739:TYR:HE1	1.64	0.46
2:B:474:LEU:CD2	2:B:514:PHE:HE1	2.22	0.45
2:F:494:ILE:H	2:F:494:ILE:HD12	1.81	0.45
1:A:305:ILE:HD13	1:A:320:LEU:HD13	1.97	0.45
1:G:402:THR:HB	1:G:405:GLU:HG3	1.98	0.45
1:A:220:ALA:O	1:A:221:ALA:HB3	2.17	0.45
2:F:701:LEU:HD23	2:F:705:ALA:CB	2.46	0.45
2:F:595:ASN:O	2:F:598:GLU:CB	2.64	0.45
1:A:35:PRO:HG3	1:A:171:SER:OG	2.16	0.45
1:E:184:PRO:HD2	1:E:217:PHE:CD1	2.51	0.45
2:F:492:SER:HA	2:F:526:HIS:O	2.16	0.45
1:C:149:TYR:O	1:C:150:ASP:C	2.54	0.45
1:C:264:ILE:CB	1:C:265:PRO:HD2	2.38	0.45
1:E:402:THR:HB	1:E:405:GLU:HG3	1.98	0.45
2:F:532:PRO:HA	2:F:754:THR:HG22	1.98	0.45
2:B:636:GLU:HA	2:B:639:ASP:OD2	2.16	0.45
2:B:470:LEU:HD12	2:B:474:LEU:HD13	1.98	0.45
1:A:165:ASN:H	1:A:168:VAL:HG23	1.81	0.45
1:C:37:VAL:HG11	1:C:345:MET:SD	2.57	0.45
2:D:495:ILE:HG21	2:D:507:ARG:HG3	1.98	0.45
2:B:515:TYR:OH	3:I:7:VAL:HG11	2.16	0.45
1:A:275:GLU:HG3	2:D:405:GLY:HA3	1.99	0.45
2:F:515:TYR:HB2	2:F:770:ALA:HB1	1.97	0.45
1:C:152:THR:O	1:C:153:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:449:LYS:HD2	2:D:461:MET:CE	2.35	0.45
1:A:161:THR:OG1	1:A:163:ILE:HG12	2.17	0.45
1:G:246:ALA:CB	1:G:317:LEU:HD11	2.47	0.45
2:F:656:GLU:HB3	2:F:657:GLN:CA	2.46	0.45
1:C:482:LEU:HA	1:C:485:ILE:HG12	1.99	0.45
1:C:191:ILE:HG21	1:C:510:ARG:HB3	1.98	0.45
2:D:516:ARG:HD3	3:K:36:ASP:OD2	2.17	0.45
2:H:403:LEU:HD22	2:H:407:LEU:HD22	1.99	0.45
2:B:531:GLN:OE1	2:B:763:LEU:HB2	2.17	0.45
1:E:441:PHE:CD2	1:E:441:PHE:N	2.85	0.45
1:C:80:HIS:HD1	3:K:56:SER:C	2.19	0.45
1:C:143:VAL:HG11	1:C:158:VAL:HB	1.98	0.45
1:G:161:THR:OG1	1:G:163:ILE:O	2.34	0.45
1:A:179:ALA:O	1:A:333:ASN:ND2	2.50	0.45
1:G:26:MET:O	1:G:30:VAL:HG23	2.17	0.45
2:B:567:HIS:HB2	2:B:706:PHE:CB	2.45	0.45
1:A:230:GLU:OE2	1:A:234:ARG:NE	2.49	0.45
1:C:111:SER:HB3	1:C:115:ASP:OD2	2.17	0.45
1:E:440:GLU:C	1:E:441:PHE:HD2	2.20	0.45
2:H:729:GLU:OE2	2:H:732:ARG:NH2	2.50	0.45
1:C:109:PHE:CE1	1:C:123:THR:HB	2.52	0.45
1:A:417:LEU:N	1:A:417:LEU:CD1	2.80	0.45
1:G:99:ARG:HG2	1:G:218:PRO:HD3	1.99	0.45
1:A:394:ILE:O	1:A:398:ARG:HB2	2.17	0.45
1:A:217:PHE:HE2	1:A:223:ILE:HD11	1.82	0.45
1:G:104:ASP:OD2	1:G:126:ARG:HD2	2.16	0.45
1:G:200:ASP:HB3	1:G:203:ILE:HG13	1.98	0.45
2:H:483:TYR:CE2	2:H:485:PRO:HG3	2.52	0.45
1:A:124:GLU:C	1:A:125:ILE:CG2	2.85	0.44
1:E:441:PHE:N	1:E:441:PHE:HD2	2.15	0.44
2:B:471:ILE:HG23	2:B:472:THR:N	2.31	0.44
2:B:567:HIS:HB2	2:B:706:PHE:HB2	1.99	0.44
1:C:212:ILE:HD12	1:C:347:LEU:HD21	1.98	0.44
2:F:546:ILE:HG21	2:F:552:MET:HA	1.98	0.44
1:A:397:ILE:HG13	1:A:406:ALA:HB1	1.99	0.44
2:B:697:LEU:HD23	2:B:697:LEU:C	2.37	0.44
2:H:765:VAL:HG23	2:H:765:VAL:O	2.18	0.44
2:H:515:TYR:CD1	2:H:515:TYR:O	2.70	0.44
1:E:497:ARG:O	1:E:501:VAL:HG23	2.17	0.44
1:E:374:ARG:HG2	1:E:485:ILE:HD12	2.00	0.44
1:A:246:ALA:HA	1:A:261:VAL:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ALA:HB2	1:E:120:MET:HG3	1.99	0.44
2:D:479:GLY:HA2	3:K:33:GLN:HE21	1.78	0.44
1:A:129:LYS:HB3	1:A:513:PHE:HE1	1.81	0.44
1:E:319:ASN:HB3	1:E:323:GLN:HE21	1.81	0.44
1:C:146:VAL:HG22	1:C:147:ASP:N	2.32	0.44
1:C:220:ALA:HB3	1:C:263:GLU:CD	2.37	0.44
2:B:667:ARG:O	2:B:667:ARG:HG2	2.18	0.44
1:A:28:VAL:HG13	1:A:29:ILE:N	2.31	0.44
2:B:408:ALA:HA	2:B:444:LEU:CD1	2.48	0.44
1:C:259:ILE:HB	1:C:305:ILE:HB	1.99	0.44
2:D:689:ARG:O	2:D:692:THR:OG1	2.30	0.44
2:F:531:GLN:HB2	2:F:761:ARG:O	2.18	0.44
3:K:28:CYS:SG	3:K:29:SER:N	2.91	0.44
2:D:422:LEU:N	2:D:494:ILE:O	2.49	0.44
1:E:471:HIS:CD2	1:E:471:HIS:C	2.91	0.44
2:F:529:ILE:HG22	2:F:530:ALA:O	2.18	0.44
1:A:164:PRO:HB2	1:A:168:VAL:CG2	2.48	0.44
1:C:24:TYR:O	1:C:24:TYR:CD1	2.70	0.44
1:G:25:ALA:HA	1:G:28:VAL:HG23	1.99	0.44
1:E:90:VAL:O	1:E:94:GLN:HG3	2.17	0.44
1:C:171:SER:OG	1:C:172:SER:N	2.51	0.44
3:L:12:CYS:SG	3:L:14:LYS:HG2	2.57	0.44
2:H:461:MET:CG	2:H:462:LEU:N	2.80	0.44
2:H:580:LEU:O	2:H:584:VAL:HG23	2.17	0.44
2:H:420:LEU:HB3	2:H:493:ILE:HD12	1.99	0.44
2:F:547:LYS:HD2	2:F:761:ARG:NH1	2.33	0.44
1:C:402:THR:HG22	1:C:404:ALA:H	1.81	0.44
2:B:662:PRO:HB2	2:B:677:LEU:HD12	1.98	0.44
1:C:152:THR:C	1:C:153:GLU:HG2	2.38	0.44
2:D:479:GLY:CA	3:K:33:GLN:HE22	2.29	0.44
2:B:448:GLY:HA3	2:B:506:ILE:HG12	1.98	0.44
1:C:264:ILE:HG12	1:C:301:MET:HE1	2.00	0.44
1:E:320:LEU:HB3	1:E:326:LEU:HD12	2.00	0.44
1:A:314:GLU:O	1:A:318:ASN:ND2	2.51	0.44
1:G:254:THR:HG22	1:G:255:GLY:N	2.33	0.43
2:F:603:LYS:CG	2:F:604:ALA:H	2.28	0.43
1:E:36:ASP:HA	1:E:337:LEU:HB2	2.00	0.43
1:A:219:THR:O	1:A:220:ALA:HB3	2.18	0.43
1:G:517:ARG:HH12	1:G:521:ILE:HD11	1.83	0.43
1:E:466:LEU:HB2	1:G:397:ILE:HG21	2.00	0.43
1:G:285:ARG:HB3	1:G:323:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:36:ASP:O	3:K:40:TRP:CD1	2.70	0.43
2:B:661:GLU:HA	2:B:662:PRO:HD3	1.82	0.43
2:B:539:LYS:O	2:B:540:GLY:C	2.56	0.43
2:B:688:ARG:O	2:B:692:THR:HG23	2.18	0.43
1:C:338:HIS:HB3	1:C:343:LYS:HD3	1.98	0.43
3:I:10:PRO:HG2	3:I:27:PHE:CE1	2.52	0.43
2:F:430:GLY:O	2:F:434:GLN:HG3	2.19	0.43
2:F:658:ASN:HB3	2:F:659:LEU:H	1.69	0.43
3:K:39:GLU:HB2	3:K:45:LYS:HE2	1.99	0.43
1:E:273:LEU:HD12	1:E:324:THR:CG2	2.48	0.43
1:C:391:ASP:N	1:C:392:PRO:HD2	2.32	0.43
2:F:661:GLU:HA	2:F:662:PRO:HD3	1.89	0.43
1:A:148:ASN:ND2	1:A:150:ASP:OD1	2.47	0.43
1:G:249:GLU:HB2	1:G:258:THR:O	2.19	0.43
3:I:41:ALA:HB3	3:J:38:GLY:HA3	2.01	0.43
1:C:254:THR:CG2	1:C:254:THR:O	2.66	0.43
1:C:237:ARG:HH21	1:C:344:ILE:HD11	1.84	0.43
2:F:419:GLU:OE2	2:F:760:ARG:NH1	2.32	0.43
2:B:641:GLU:OE2	2:B:645:SER:HB3	2.18	0.43
2:B:496:MET:HG2	2:B:742:LEU:HD21	2.00	0.43
1:G:70:VAL:HG13	1:G:85:VAL:HB	2.00	0.43
1:A:183:PRO:HG3	1:A:330:PHE:CE1	2.54	0.43
3:L:12:CYS:SG	3:L:14:LYS:CG	3.06	0.43
1:C:223:ILE:HG21	1:C:229:ILE:HD11	2.00	0.43
1:E:222:ILE:HG22	1:E:223:ILE:N	2.34	0.43
2:D:520:GLU:O	2:D:524:ARG:HG2	2.18	0.43
2:H:523:GLU:C	2:H:525:GLY:N	2.70	0.43
2:D:478:ILE:HD13	3:K:37:LEU:HD23	1.99	0.43
1:C:387:LEU:HA	1:C:390:ILE:HD11	2.01	0.43
2:F:746:ASN:HB2	2:F:749:GLN:HG3	1.99	0.43
2:B:538:LYS:HA	2:B:542:GLN:O	2.19	0.43
2:D:583:LEU:HD21	2:D:719:PHE:HZ	1.83	0.43
2:H:753:THR:OG1	2:H:754:THR:HG23	2.19	0.43
1:E:443:VAL:O	1:E:444:ARG:C	2.57	0.43
3:L:17:VAL:HG13	3:L:17:VAL:O	2.18	0.43
1:G:58:ASP:OD1	1:G:58:ASP:N	2.51	0.43
1:A:475:LEU:O	1:A:478:TYR:N	2.51	0.42
2:H:424:GLU:OE1	2:H:498:ASP:HB2	2.19	0.42
2:F:701:LEU:N	2:F:701:LEU:HD12	2.34	0.42
1:A:183:PRO:HB2	1:A:215:PRO:HB3	2.00	0.42
1:E:464:GLN:HG3	1:G:459:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:383:LEU:O	1:G:387:LEU:HG	2.19	0.42
1:E:337:LEU:HD23	1:E:337:LEU:HA	1.88	0.42
2:F:750:LEU:O	2:F:754:THR:OG1	2.27	0.42
2:B:544:GLN:HG2	2:B:545:TYR:N	2.34	0.42
1:C:100:TYR:HD2	1:C:168:VAL:HG13	1.84	0.42
2:F:659:LEU:HD22	2:F:679:HIS:CD2	2.54	0.42
2:F:656:GLU:CB	2:F:657:GLN:CA	2.91	0.42
1:C:274:ILE:HD13	1:C:294:ASP:HB2	2.00	0.42
1:A:158:VAL:HG12	1:A:159:MET:N	2.35	0.42
1:E:469:LEU:CD1	1:E:473:LYS:HG3	2.49	0.42
1:C:387:LEU:HB3	1:C:471:HIS:CE1	2.55	0.42
1:E:186:ASN:ND2	1:E:515:ASP:O	2.43	0.42
1:C:221:ALA:H	1:C:519:THR:HG22	1.84	0.42
1:E:51:ALA:O	1:E:55:LEU:HD13	2.19	0.42
1:C:20:SER:OG	1:C:21:TYR:N	2.50	0.42
2:D:424:GLU:HB3	2:D:427:SER:HB3	2.01	0.42
2:H:528:TYR:OH	2:H:764:ARG:NH2	2.52	0.42
1:A:203:ILE:HG12	1:A:204:SER:H	1.83	0.42
1:C:220:ALA:O	1:C:263:GLU:HB3	2.19	0.42
1:A:519:THR:HG23	1:A:519:THR:O	2.19	0.42
1:E:274:ILE:HD13	1:E:294:ASP:HB2	2.01	0.42
2:F:610:ILE:CD1	2:F:611:TYR:CD1	3.02	0.42
1:C:59:TRP:HD1	1:C:132:HIS:ND1	2.17	0.42
1:A:245:ARG:HG3	1:A:245:ARG:O	2.20	0.42
1:A:450:LEU:HD11	1:A:454:GLN:HB2	2.01	0.42
1:A:414:PRO:CA	1:A:448:TYR:O	2.68	0.42
1:A:315:VAL:HA	1:E:319:ASN:ND2	2.34	0.42
1:G:220:ALA:O	1:G:263:GLU:HB3	2.18	0.42
1:C:497:ARG:HA	1:C:497:ARG:HD2	1.88	0.42
1:A:186:ASN:HB2	1:A:216:ASP:OD2	2.20	0.42
2:F:657:GLN:O	2:F:657:GLN:CG	2.62	0.42
1:A:341:GLN:HA	1:A:342:PRO:HD3	1.83	0.42
2:H:432:ALA:HB1	2:H:443:ILE:HD12	2.00	0.42
2:D:769:ASP:OD1	2:D:769:ASP:N	2.53	0.42
1:C:76:LYS:HB2	1:C:77:TYR:CD1	2.55	0.42
1:A:21:TYR:O	1:A:22:LEU:C	2.58	0.42
2:D:403:LEU:N	2:D:404:PRO:HD2	2.32	0.42
2:B:609:LEU:HG	2:B:687:TYR:HE1	1.84	0.42
2:F:537:VAL:HG11	2:F:546:ILE:HD11	2.00	0.42
1:A:182:ILE:HG12	1:A:334:MET:HA	2.02	0.42
1:A:442:GLY:O	1:A:449:TYR:N	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:566:LEU:HD23	2:F:575:LEU:HD23	2.02	0.42
2:H:591:GLN:O	2:H:594:ILE:HG13	2.19	0.42
2:D:493:ILE:HD11	2:D:527:VAL:HG12	2.01	0.42
2:B:408:ALA:HA	2:B:444:LEU:HD13	2.01	0.42
2:B:715:PRO:C	2:B:716:VAL:CG1	2.88	0.42
2:F:559:ILE:HD13	2:F:559:ILE:HA	1.89	0.42
1:G:400:ALA:HA	1:G:401:PRO:HD3	1.80	0.42
1:G:358:ARG:HA	1:G:358:ARG:HD2	1.81	0.42
2:B:516:ARG:NH1	3:I:45:LYS:HZ2	2.17	0.42
2:F:595:ASN:HA	2:F:598:GLU:HB2	2.02	0.42
1:G:355:VAL:O	1:G:359:ARG:HG3	2.20	0.42
2:F:580:LEU:O	2:F:584:VAL:HG23	2.20	0.42
2:F:593:MET:SD	2:F:686:GLU:HG3	2.60	0.42
2:H:423:VAL:HG23	2:H:445:PRO:HA	2.02	0.42
2:D:547:LYS:HG3	2:D:548:ASP:H	1.85	0.42
2:F:517:GLN:NE2	3:J:33:GLN:OE1	2.53	0.42
2:B:497:THR:CG2	2:B:503:GLY:O	2.67	0.42
1:C:233:TYR:HD1	1:C:347:LEU:HB2	1.85	0.42
2:D:409:ASP:OD2	2:D:489:ARG:NH2	2.53	0.42
3:K:58:ASP:OD1	3:K:59:TRP:N	2.53	0.41
1:E:443:VAL:O	1:E:446:GLY:N	2.53	0.41
1:A:358:ARG:HA	1:A:358:ARG:HD2	1.89	0.41
1:C:400:ALA:HA	1:C:401:PRO:HD3	1.87	0.41
1:C:517:ARG:HH21	1:C:521:ILE:HD11	1.84	0.41
1:G:356:ARG:HG3	1:G:359:ARG:HH21	1.83	0.41
2:F:436:ARG:HH12	1:G:295:GLU:HA	1.85	0.41
1:C:253:LYS:HG3	1:C:253:LYS:O	2.20	0.41
1:E:380:LEU:HD11	1:E:477:GLU:CD	2.39	0.41
2:H:509:LEU:CD1	3:L:47:ILE:CD1	2.87	0.41
1:A:247:GLU:O	1:A:260:ILE:N	2.53	0.41
2:B:548:ASP:HB2	2:B:549:ASP:H	1.71	0.41
1:E:469:LEU:O	1:E:469:LEU:HD22	2.20	0.41
1:C:478:TYR:CE2	1:C:482:LEU:HD11	2.55	0.41
1:C:173:GLY:N	1:C:180:THR:O	2.52	0.41
1:C:182:ILE:HA	1:C:183:PRO:HD3	1.80	0.41
1:E:142:THR:C	1:E:364:ARG:HH11	2.24	0.41
2:H:422:LEU:HD23	2:H:444:LEU:HB3	2.03	0.41
1:A:471:HIS:NE2	1:A:475:LEU:CD1	2.73	0.41
1:C:245:ARG:CG	1:C:245:ARG:HH11	2.19	0.41
1:E:462:ARG:NH2	1:G:460:ASP:OD1	2.52	0.41
1:C:382:ALA:HB2	1:C:454:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:HIS:C	1:C:263:GLU:HG3	2.40	0.41
2:B:703:GLU:O	2:B:704:ASP:HB2	2.19	0.41
2:B:539:LYS:HB2	2:B:734:LEU:HD23	2.01	0.41
2:B:528:TYR:HE2	2:B:764:ARG:NE	2.17	0.41
2:F:478:ILE:O	2:F:482:GLU:HB2	2.21	0.41
2:F:505:HIS:O	2:F:509:LEU:HG	2.20	0.41
2:F:623:GLU:HB2	2:F:660:PHE:CE2	2.54	0.41
2:B:556:GLN:CD	2:B:731:ARG:HH12	2.24	0.41
1:C:310:ASP:OD1	1:C:310:ASP:N	2.53	0.41
2:B:471:ILE:CG2	2:B:472:THR:N	2.84	0.41
1:E:186:ASN:HB2	1:E:216:ASP:OD2	2.21	0.41
2:D:510:LEU:HD23	2:D:510:LEU:HA	1.74	0.41
3:K:35:ILE:O	3:K:39:GLU:HG3	2.20	0.41
1:G:419:ASN:C	1:G:420:VAL:HG22	2.41	0.41
1:E:182:ILE:HA	1:E:183:PRO:HD3	1.83	0.41
1:C:507:GLU:HA	1:C:510:ARG:HG2	2.01	0.41
1:G:347:LEU:O	1:G:351:ILE:HG12	2.19	0.41
1:C:91:ARG:HA	1:C:94:GLN:HE21	1.85	0.41
1:A:142:THR:O	1:A:364:ARG:HD3	2.21	0.41
1:E:163:ILE:HA	1:E:164:PRO:HD2	1.92	0.41
1:C:73:VAL:O	1:C:78:HIS:N	2.48	0.41
2:B:528:TYR:HE2	2:B:764:ARG:CZ	2.33	0.41
2:H:415:PRO:O	2:H:491:HIS:HB2	2.20	0.41
2:H:772:ALA:O	2:H:775:GLN:HG2	2.21	0.41
3:K:25:ARG:HA	3:K:26:PRO:HA	1.87	0.41
1:G:113:ASP:HB2	1:G:115:ASP:OD2	2.20	0.41
2:H:422:LEU:HA	2:H:444:LEU:O	2.21	0.41
1:A:423:MET:O	1:A:424:LEU:C	2.59	0.41
1:G:363:THR:O	1:G:367:ILE:HG13	2.21	0.41
1:G:178:MET:SD	1:G:178:MET:N	2.94	0.41
2:B:502:ASP:O	2:B:505:HIS:HB2	2.20	0.41
1:A:189:GLU:OE2	1:A:517:ARG:HD2	2.21	0.41
1:G:383:LEU:HD22	1:G:461:LEU:HD12	2.03	0.41
2:F:626:VAL:HG13	2:F:662:PRO:HG3	2.01	0.41
2:D:689:ARG:HG3	2:D:690:ILE:H	1.85	0.41
1:E:511:GLU:OE2	1:E:511:GLU:HA	2.21	0.41
2:H:727:VAL:O	2:H:731:ARG:HG2	2.21	0.41
1:G:259:ILE:HG13	1:G:307:VAL:CG2	2.51	0.41
1:A:482:LEU:HA	1:A:485:ILE:HG12	2.02	0.41
2:B:719:PHE:O	2:B:722:ALA:N	2.54	0.41
2:B:452:ASN:CB	2:B:460:LYS:HZ2	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:464:GLN:HB2	1:G:459:LEU:HB3	2.03	0.41
1:C:185:HIS:CD2	1:C:215:PRO:HA	2.56	0.41
2:F:404:PRO:HG2	2:F:405:GLY:H	1.85	0.41
1:E:242:ILE:HD11	1:E:330:PHE:HB2	2.03	0.41
1:E:524:ASN:N	1:E:524:ASN:OD1	2.54	0.41
1:A:37:VAL:H	1:A:37:VAL:HG12	1.56	0.41
2:H:523:GLU:C	2:H:525:GLY:H	2.24	0.40
3:K:42:ALA:C	3:K:43:GLU:HG3	2.42	0.40
1:C:30:VAL:HG13	1:C:34:LEU:CD1	2.39	0.40
2:D:527:VAL:O	2:D:527:VAL:HG23	2.20	0.40
1:A:217:PHE:CE2	1:A:223:ILE:HD11	2.56	0.40
2:F:524:ARG:HB2	2:F:526:HIS:CD2	2.56	0.40
1:G:285:ARG:HB3	1:G:323:GLN:NE2	2.37	0.40
1:A:245:ARG:NH1	1:A:520:GLU:OE1	2.51	0.40
1:A:370:LEU:O	1:A:374:ARG:HG2	2.21	0.40
1:A:374:ARG:HD3	1:A:374:ARG:HA	1.82	0.40
1:G:93:ALA:HA	1:G:103:VAL:O	2.21	0.40
1:A:491:ILE:HD11	1:A:497:ARG:HE	1.86	0.40
1:A:503:ARG:NH1	1:A:503:ARG:HB3	2.35	0.40
1:C:250:VAL:HA	1:C:256:ARG:O	2.22	0.40
1:G:262:HIS:O	1:G:301:MET:HG3	2.21	0.40
2:F:691:CYS:O	2:F:695:GLU:HG3	2.20	0.40
1:A:310:ASP:OD1	1:A:310:ASP:N	2.53	0.40
3:K:36:ASP:OD1	3:K:45:LYS:HE3	2.20	0.40
1:A:221:ALA:N	1:A:263:GLU:OE2	2.46	0.40
1:A:508:LEU:O	1:A:512:GLN:HG3	2.22	0.40
1:E:522:THR:HG22	1:E:523:ALA:N	2.36	0.40
2:B:663:ILE:HG12	2:B:676:PRO:HA	2.02	0.40
2:D:493:ILE:CG1	2:D:527:VAL:HG12	2.52	0.40
1:A:230:GLU:CD	1:A:234:ARG:HE	2.25	0.40
1:A:47:ARG:HA	1:A:155:ILE:HD11	2.04	0.40
1:A:28:VAL:CG1	1:A:29:ILE:N	2.85	0.40
1:A:65:LYS:O	1:A:67:ALA:N	2.54	0.40
1:E:465:LYS:HA	1:E:470:GLU:HG3	2.03	0.40
1:E:358:ARG:HH12	1:E:361:VAL:HG11	1.87	0.40
2:D:547:LYS:HB3	2:D:761:ARG:NH1	2.37	0.40
2:F:742:LEU:HA	2:F:742:LEU:HD23	1.82	0.40
1:A:376:ARG:O	1:A:380:LEU:HB2	2.21	0.40
2:D:451:LEU:HD23	2:D:451:LEU:HA	1.96	0.40
2:B:420:LEU:O	2:B:493:ILE:HA	2.21	0.40

All (16) 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)
1:E:476:ASP:OD2	2:F:596:ARG:CZ[3_757]	1.27	0.93
1:E:476:ASP:OD2	2:F:596:ARG:NE[3_757]	1.27	0.93
1:E:476:ASP:CG	2:F:596:ARG:NE[3_757]	1.32	0.88
1:E:476:ASP:CG	2:F:596:ARG:CZ[3_757]	1.33	0.87
1:E:476:ASP:CG	2:F:596:ARG:NH2[3_757]	1.39	0.81
1:E:476:ASP:CB	2:F:596:ARG:NH2[3_757]	1.40	0.80
1:E:476:ASP:CB	2:F:596:ARG:CZ[3_757]	1.49	0.71
1:E:473:LYS:NZ	2:F:597:MET:CA[3_757]	1.59	0.61
1:E:473:LYS:NZ	2:F:596:ARG:O[3_757]	1.60	0.60
1:E:476:ASP:OD2	2:F:596:ARG:NH2[3_757]	1.61	0.59
1:E:473:LYS:NZ	2:F:597:MET:N[3_757]	1.74	0.46
1:E:473:LYS:NZ	2:F:596:ARG:C[3_757]	1.77	0.43
1:E:476:ASP:OD1	2:F:596:ARG:NE[3_757]	2.01	0.19
1:E:473:LYS:CE	2:F:596:ARG:O[3_757]	2.12	0.08
1:A:511:GLU:OE1	2:B:573:PRO:O[4_477]	2.13	0.07
1:C:314:GLU:OE1	2:H:491:HIS:ND1[1_545]	2.13	0.07

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	497/525 (95%)	473 (95%)	22 (4%)	2 (0%)	39 76
1	C	469/525 (89%)	438 (93%)	30 (6%)	1 (0%)	52 85
1	E	477/525 (91%)	454 (95%)	22 (5%)	1 (0%)	52 85
1	G	475/525 (90%)	443 (93%)	31 (6%)	1 (0%)	52 85
2	B	370/417 (89%)	341 (92%)	28 (8%)	1 (0%)	46 81
2	D	239/417 (57%)	225 (94%)	13 (5%)	1 (0%)	39 76
2	F	365/417 (88%)	347 (95%)	18 (5%)	0	100 100
2	H	224/417 (54%)	206 (92%)	17 (8%)	1 (0%)	39 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	45/65 (69%)	42 (93%)	3 (7%)	0	100	100
3	J	53/65 (82%)	50 (94%)	3 (6%)	0	100	100
3	K	51/65 (78%)	47 (92%)	4 (8%)	0	100	100
3	L	46/65 (71%)	46 (100%)	0	0	100	100
All	All	3311/4028 (82%)	3112 (94%)	191 (6%)	8 (0%)	52	85

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ALA
1	E	401	PRO
2	B	696	LYS
1	A	136	ALA
1	G	439	PRO
2	H	524	ARG
1	C	79	PRO
2	D	403	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/440 (96%)	406 (96%)	16 (4%)	40	75
1	C	397/440 (90%)	387 (98%)	10 (2%)	55	82
1	E	407/440 (92%)	397 (98%)	10 (2%)	55	82
1	G	403/440 (92%)	387 (96%)	16 (4%)	38	74
2	B	322/352 (92%)	306 (95%)	16 (5%)	30	68
2	D	214/352 (61%)	207 (97%)	7 (3%)	45	78
2	F	319/352 (91%)	311 (98%)	8 (2%)	55	82
2	H	202/352 (57%)	196 (97%)	6 (3%)	48	79
3	I	41/59 (70%)	40 (98%)	1 (2%)	57	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	J	51/59 (86%)	48 (94%)	3 (6%)	24 63
3	K	49/59 (83%)	47 (96%)	2 (4%)	37 74
3	L	42/59 (71%)	41 (98%)	1 (2%)	57 83
All	All	2869/3404 (84%)	2773 (97%)	96 (3%)	45 78

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ASP
1	A	101	MET
1	A	108	ASN
1	A	124	GLU
1	A	134	LEU
1	A	341	GLN
1	A	355	VAL
1	A	443	VAL
1	A	458	ILE
1	A	460	ASP
1	A	470	GLU
1	A	482	LEU
1	A	491	ILE
1	A	513	PHE
1	A	517	ARG
1	A	522	THR
2	B	460	LYS
2	B	469	THR
2	B	481	ASP
2	B	492	SER
2	B	498	ASP
2	B	500	ASP
2	B	528	TYR
2	B	529	ILE
2	B	546	ILE
2	B	548	ASP
2	B	566	LEU
2	B	652	HIS
2	B	668	THR
2	B	702	GLU
2	B	706	PHE
2	B	723	LEU
1	C	121	ARG

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Mol	Chain	Res	Type
1	C	149	TYR
1	C	168	VAL
1	C	180	THR
1	C	201	GLU
1	C	310	ASP
1	C	323	GLN
1	C	332	ILE
1	C	338	HIS
1	C	391	ASP
2	D	426	ASP
2	D	463	SER
2	D	719	PHE
2	D	734	LEU
2	D	765	VAL
2	D	769	ASP
2	D	777	PHE
1	E	130	ILE
1	E	174	ILE
1	E	201	GLU
1	E	272[A]	ARG
1	E	272[B]	ARG
1	E	292	LEU
1	E	328	VAL
1	E	482	LEU
1	E	496	ASP
1	E	517	ARG
2	F	409	ASP
2	F	450	ILE
2	F	550	GLU
2	F	609	LEU
2	F	610	ILE
2	F	661	GLU
2	F	683	THR
2	F	775	GLN
1	G	24	TYR
1	G	27	SER
1	G	32	ARG
1	G	58	ASP
1	G	72	ASP
1	G	121	ARG
1	G	124	GLU
1	G	178	MET

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Mol	Chain	Res	Type
1	G	202	ASP
1	G	275	GLU
1	G	338	HIS
1	G	345	MET
1	G	419	ASN
1	G	469	LEU
1	G	471	HIS
1	G	517	ARG
2	H	423	VAL
2	H	449	LYS
2	H	482	GLU
2	H	492	SER
2	H	498	ASP
2	H	587	TYR
3	I	50	SER
3	J	33	GLN
3	J	57	ASP
3	J	58	ASP
3	K	37	LEU
3	K	45	LYS
3	L	24	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	378	HIS
1	A	464	GLN
2	B	526	HIS
2	B	542	GLN
2	B	556	GLN
2	B	624	GLN
2	B	737	GLN
2	B	749	GLN
1	C	94	GLN
1	C	106	GLN
1	C	454	GLN
1	C	464	GLN
2	D	411	GLN
2	D	434	GLN
2	D	517	GLN
2	D	531	GLN

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Mol	Chain	Res	Type
2	D	749	GLN
2	D	775	GLN
1	E	45	HIS
1	E	319	ASN
1	E	471	HIS
1	E	484	GLN
1	E	512	GLN
2	F	517	GLN
2	F	624	GLN
2	F	679	HIS
2	F	737	GLN
1	G	57	ASN
1	G	106	GLN
1	G	267	GLN
1	G	323	GLN
1	G	338	HIS
1	G	453	GLN
1	G	484	GLN
2	H	544	GLN
2	H	556	GLN
2	H	746	ASN
2	H	749	GLN
3	J	33	GLN
3	K	33	GLN
3	L	8	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	505/525 (96%)	-0.00	14 (2%) 56 50	67, 110, 249, 473	0
1	C	475/525 (90%)	0.13	26 (5%) 29 23	75, 145, 252, 431	0
1	E	486/525 (92%)	0.01	16 (3%) 50 43	65, 104, 254, 314	0
1	G	483/525 (92%)	0.04	16 (3%) 50 43	59, 139, 235, 370	0
2	B	374/417 (89%)	-0.09	4 (1%) 82 78	69, 132, 176, 208	0
2	D	251/417 (60%)	0.30	19 (7%) 17 14	86, 145, 270, 299	0
2	F	371/417 (88%)	0.01	5 (1%) 79 74	59, 121, 200, 247	0
2	H	233/417 (55%)	0.23	18 (7%) 16 13	79, 132, 263, 362	0
3	I	47/65 (72%)	-0.33	0 100 100	65, 106, 140, 149	0
3	J	57/65 (87%)	-0.07	2 (3%) 48 40	66, 108, 144, 153	0
3	K	55/65 (84%)	0.50	6 (10%) 7 6	136, 176, 205, 211	0
3	L	48/65 (73%)	0.13	2 (4%) 40 33	166, 194, 227, 283	0
All	All	3385/4028 (84%)	0.06	128 (3%) 44 37	59, 130, 246, 473	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	386	ALA	8.4
2	D	719	PHE	8.1
1	A	385	VAL	7.6
1	A	17	LEU	6.4
3	K	51	GLY	5.8
1	C	194	CYS	5.6
1	C	463	LEU	5.3
1	A	386	ALA	5.3
1	C	387	LEU	4.8
2	H	584	VAL	4.7
2	D	588	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	386	ALA	4.3
2	H	581	GLU	4.3
2	H	730	SER	4.2
1	E	443	VAL	4.2
1	E	26	MET	4.2
1	E	385	VAL	4.2
1	E	466	LEU	4.1
1	E	29	ILE	4.0
1	A	383	LEU	4.0
3	L	40	TRP	3.9
1	G	466	LEU	3.9
1	C	466	LEU	3.8
1	C	381	GLU	3.8
1	G	393	ILE	3.7
1	A	466	LEU	3.7
2	H	513	PHE	3.7
2	H	729	GLU	3.7
2	H	561	LEU	3.6
1	G	521	ILE	3.5
2	D	688	ARG	3.5
2	H	478	ILE	3.5
1	C	313	GLY	3.4
1	C	383	LEU	3.4
2	D	561	LEU	3.4
1	G	215	PRO	3.4
1	C	384	ALA	3.4
2	H	586	GLU	3.3
1	A	405	GLU	3.3
1	C	397	ILE	3.3
1	E	426	ARG	3.3
2	D	718	SER	3.2
3	L	18	TRP	3.2
2	F	662	PRO	3.2
2	H	562	ASP	3.2
1	C	377	ALA	3.2
1	A	397	ILE	3.2
1	A	436	TRP	3.1
1	G	198	ILE	3.1
1	C	317	LEU	3.1
1	C	492	LEU	3.1
1	C	385	VAL	3.1
2	H	481	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	428	GLY	3.1
1	A	465	LYS	3.0
1	A	19	SER	3.0
2	D	731	ARG	3.0
1	G	513	PHE	3.0
1	G	481	LEU	3.0
2	B	783	ASP	3.0
2	H	588	ASN	3.0
3	K	6	THR	2.9
1	C	318	ASN	2.9
2	H	726	LEU	2.8
1	A	470	GLU	2.8
1	G	383	LEU	2.8
2	H	590	THR	2.8
3	J	4	THR	2.8
3	K	26	PRO	2.8
2	D	690	ILE	2.7
2	D	691	CYS	2.7
1	E	178	MET	2.7
2	B	649	PHE	2.7
1	G	194	CYS	2.6
2	F	716	VAL	2.6
1	A	393	ILE	2.6
1	E	387	LEU	2.6
2	D	590	THR	2.6
1	G	465	LYS	2.5
2	D	593	MET	2.5
1	C	420	VAL	2.5
1	C	464	GLN	2.5
2	B	474	LEU	2.5
2	D	722	ALA	2.5
2	H	585	SER	2.5
2	B	445	PRO	2.5
1	C	488	LEU	2.4
2	D	729	GLU	2.4
3	K	7	VAL	2.4
1	E	425	GLU	2.4
1	G	164	PRO	2.4
1	E	393	ILE	2.4
3	K	18	TRP	2.4
3	J	56	SER	2.3
1	C	382	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	677	LEU	2.3
2	D	589	ALA	2.3
1	C	286	VAL	2.2
2	D	587	TYR	2.2
1	G	397	ILE	2.2
2	H	558	SER	2.2
2	H	592	LYS	2.2
2	D	562	ASP	2.2
1	C	320	LEU	2.2
1	C	233	TYR	2.2
2	D	687	TYR	2.2
1	E	384	ALA	2.2
2	F	646	GLN	2.1
2	D	478	ILE	2.1
1	C	167	LEU	2.1
3	K	63	PRO	2.1
1	A	388	ALA	2.1
1	E	397	ILE	2.1
1	G	214	GLY	2.1
1	A	384	ALA	2.1
1	G	26	MET	2.1
2	D	534	LEU	2.1
2	H	583	LEU	2.1
2	H	594	ILE	2.0
1	E	176	VAL	2.0
1	C	410	LEU	2.0
1	C	190	VAL	2.0
1	G	498	LEU	2.0
1	E	177	GLY	2.0
1	G	27	SER	2.0
2	D	734	LEU	2.0
1	C	289	ILE	2.0
2	F	575	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	ZN	E	601	1/1	0.76	0.27	1.12	346,346,346,346	0
4	ZN	I	101	1/1	0.97	0.16	0.32	95,95,95,95	0
4	ZN	L	101	1/1	0.80	0.14	-0.99	225,225,225,225	0
4	ZN	K	101	1/1	0.71	0.11	-1.17	202,202,202,202	0
4	ZN	J	101	1/1	0.99	0.10	-1.36	137,137,137,137	0
4	ZN	B	1001	1/1	0.83	0.54	-	346,346,346,346	0

6.5 Other polymers

There are no such residues in this entry.