Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2017 – 05:29 am GMT

PDB ID	:	4AB7
Title	:	Crystal structure of a tetrameric acetylglutamate kinase from Saccharomyces cerevisiae complexed with its substrate N- acetylglutamate
Authors	:	De Cima, S.; Gil-Ortiz, F.; Crabeel, M.; Fita, I.; Rubio, V.
Deposited on	:	2011-12-07
Resolution	:	3.25 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:

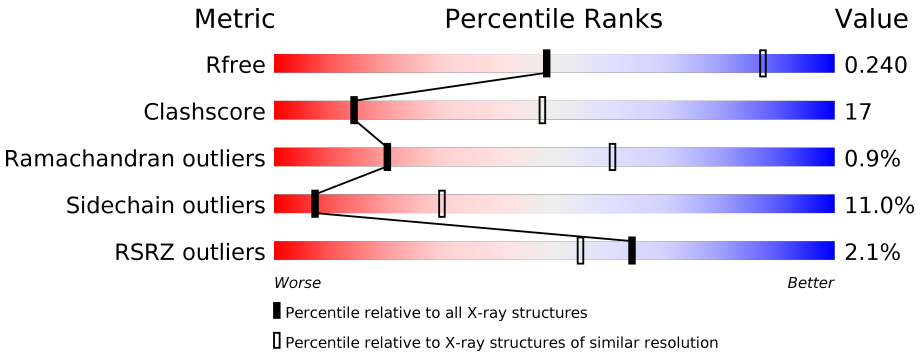
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 3.25 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}	100719	1852 (3.32-3.20)
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)
RSRZ outliers	101464	1861 (3.32-3.20)

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	464	61% 22% • • 13%
1	B	464	2% 60% 30% • 6%
1	C	464	2% 59% 31% • • 6%
1	D	464	% 61% 22% • 13%
1	E	464	4% 62% 21% • 13%
1	F	464	% 61% 28% 5% 6%

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Mol	Chain	Length	Quality of chain
1	G	464	5% 61% 27% 6% 6%
1	H	464	2% 58% 29% 9%

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
2	NLG	D	1503	-	-	X	-
2	NLG	H	1503	-	-	-	X

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 26320 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 PROTEIN ARG5,6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3140	2002	525	604	9			
1	B	436	Total	C	N	O	S	0	0	0
			3400	2164	572	655	9			
1	C	436	Total	C	N	O	S	0	0	0
			3394	2161	569	655	9			
1	D	405	Total	C	N	O	S	0	0	0
			3140	2002	525	604	9			
1	E	405	Total	C	N	O	S	0	0	0
			3142	2002	527	604	9			
1	F	436	Total	C	N	O	S	0	0	0
			3402	2167	571	655	9			
1	G	436	Total	C	N	O	S	0	0	0
			3396	2161	571	655	9			
1	H	422	Total	C	N	O	S	0	0	0
			3280	2093	547	631	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	EXPRESSION TAG	UNP Q01217
A	51	GLY	-	EXPRESSION TAG	UNP Q01217
A	52	HIS	-	EXPRESSION TAG	UNP Q01217
A	53	HIS	-	EXPRESSION TAG	UNP Q01217
A	54	HIS	-	EXPRESSION TAG	UNP Q01217
A	55	HIS	-	EXPRESSION TAG	UNP Q01217
A	56	HIS	-	EXPRESSION TAG	UNP Q01217
A	57	HIS	-	EXPRESSION TAG	UNP Q01217
B	50	MET	-	EXPRESSION TAG	UNP Q01217
B	51	GLY	-	EXPRESSION TAG	UNP Q01217
B	52	HIS	-	EXPRESSION TAG	UNP Q01217
B	53	HIS	-	EXPRESSION TAG	UNP Q01217
B	54	HIS	-	EXPRESSION TAG	UNP Q01217

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Chain	Residue	Modelled	Actual	Comment	Reference
B	55	HIS	-	EXPRESSION TAG	UNP Q01217
B	56	HIS	-	EXPRESSION TAG	UNP Q01217
B	57	HIS	-	EXPRESSION TAG	UNP Q01217
C	50	MET	-	EXPRESSION TAG	UNP Q01217
C	51	GLY	-	EXPRESSION TAG	UNP Q01217
C	52	HIS	-	EXPRESSION TAG	UNP Q01217
C	53	HIS	-	EXPRESSION TAG	UNP Q01217
C	54	HIS	-	EXPRESSION TAG	UNP Q01217
C	55	HIS	-	EXPRESSION TAG	UNP Q01217
C	56	HIS	-	EXPRESSION TAG	UNP Q01217
C	57	HIS	-	EXPRESSION TAG	UNP Q01217
D	50	MET	-	EXPRESSION TAG	UNP Q01217
D	51	GLY	-	EXPRESSION TAG	UNP Q01217
D	52	HIS	-	EXPRESSION TAG	UNP Q01217
D	53	HIS	-	EXPRESSION TAG	UNP Q01217
D	54	HIS	-	EXPRESSION TAG	UNP Q01217
D	55	HIS	-	EXPRESSION TAG	UNP Q01217
D	56	HIS	-	EXPRESSION TAG	UNP Q01217
D	57	HIS	-	EXPRESSION TAG	UNP Q01217
E	50	MET	-	EXPRESSION TAG	UNP Q01217
E	51	GLY	-	EXPRESSION TAG	UNP Q01217
E	52	HIS	-	EXPRESSION TAG	UNP Q01217
E	53	HIS	-	EXPRESSION TAG	UNP Q01217
E	54	HIS	-	EXPRESSION TAG	UNP Q01217
E	55	HIS	-	EXPRESSION TAG	UNP Q01217
E	56	HIS	-	EXPRESSION TAG	UNP Q01217
E	57	HIS	-	EXPRESSION TAG	UNP Q01217
F	50	MET	-	EXPRESSION TAG	UNP Q01217
F	51	GLY	-	EXPRESSION TAG	UNP Q01217
F	52	HIS	-	EXPRESSION TAG	UNP Q01217
F	53	HIS	-	EXPRESSION TAG	UNP Q01217
F	54	HIS	-	EXPRESSION TAG	UNP Q01217
F	55	HIS	-	EXPRESSION TAG	UNP Q01217
F	56	HIS	-	EXPRESSION TAG	UNP Q01217
F	57	HIS	-	EXPRESSION TAG	UNP Q01217
G	50	MET	-	EXPRESSION TAG	UNP Q01217
G	51	GLY	-	EXPRESSION TAG	UNP Q01217
G	52	HIS	-	EXPRESSION TAG	UNP Q01217
G	53	HIS	-	EXPRESSION TAG	UNP Q01217
G	54	HIS	-	EXPRESSION TAG	UNP Q01217
G	55	HIS	-	EXPRESSION TAG	UNP Q01217
G	56	HIS	-	EXPRESSION TAG	UNP Q01217

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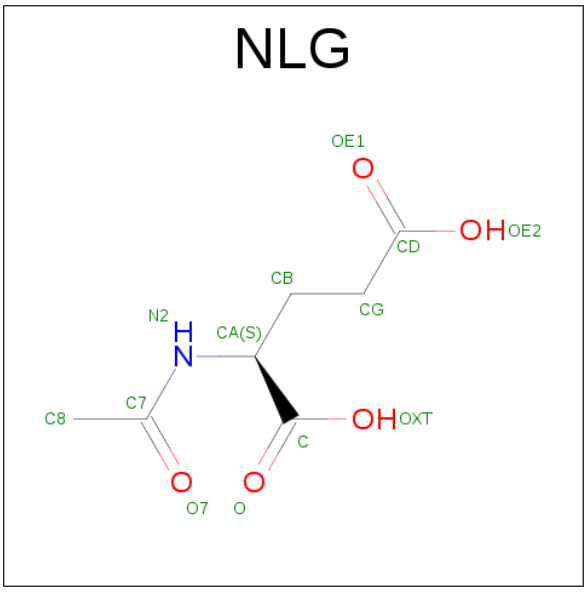
Chain	Residue	Modelled	Actual	Comment	Reference
G	57	HIS	-	EXPRESSION TAG	UNP Q01217
H	50	MET	-	EXPRESSION TAG	UNP Q01217
H	51	GLY	-	EXPRESSION TAG	UNP Q01217
H	52	HIS	-	EXPRESSION TAG	UNP Q01217
H	53	HIS	-	EXPRESSION TAG	UNP Q01217
H	54	HIS	-	EXPRESSION TAG	UNP Q01217
H	55	HIS	-	EXPRESSION TAG	UNP Q01217
H	56	HIS	-	EXPRESSION TAG	UNP Q01217
H	57	HIS	-	EXPRESSION TAG	UNP Q01217

- Molecule 2 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula: $C_7H_{11}NO_5$).



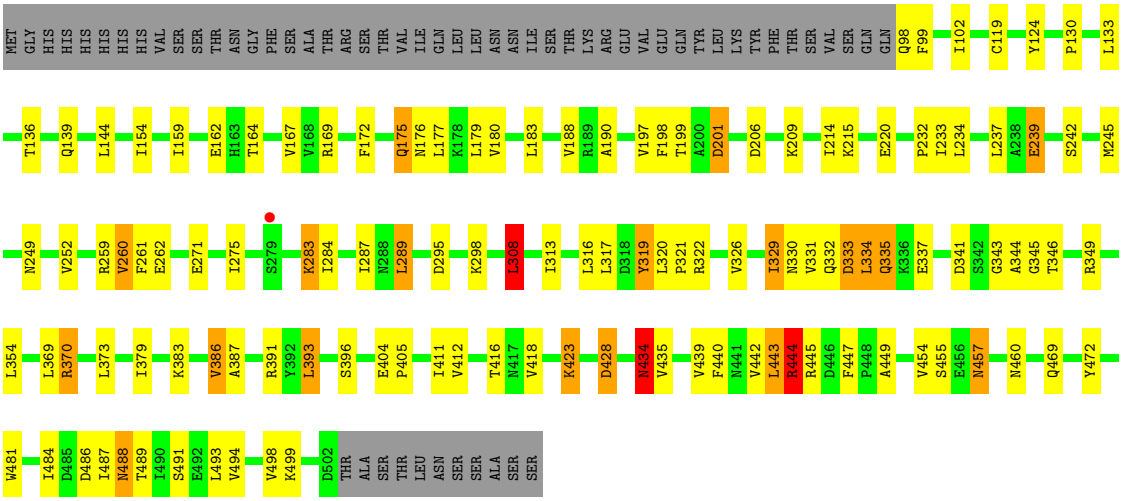
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C N O 13 7 1 5	0	0
2	H	1	Total C N O 13 7 1 5	0	0

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

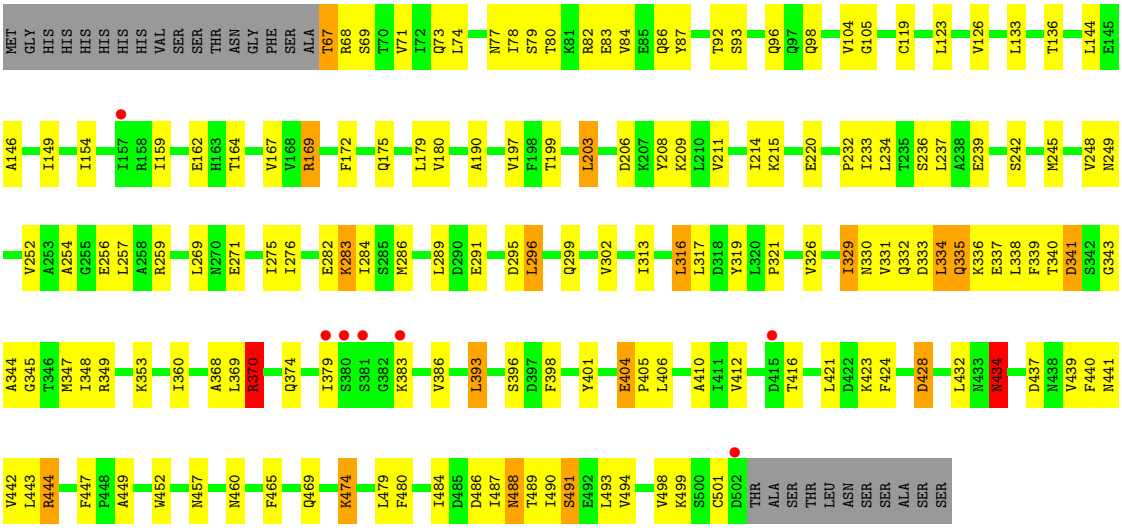
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain A:



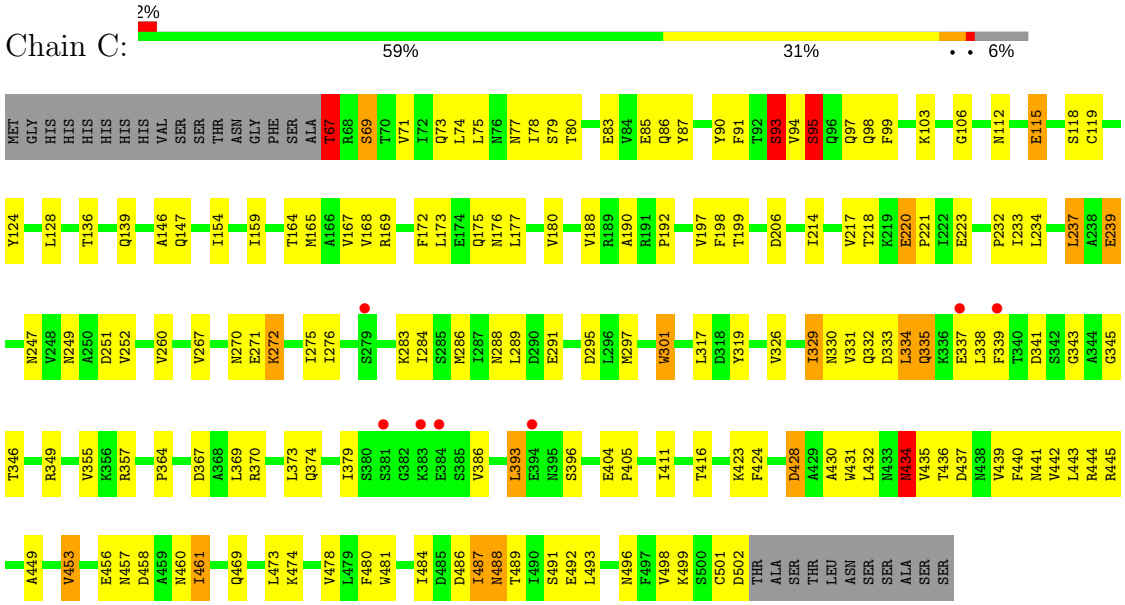
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain B:



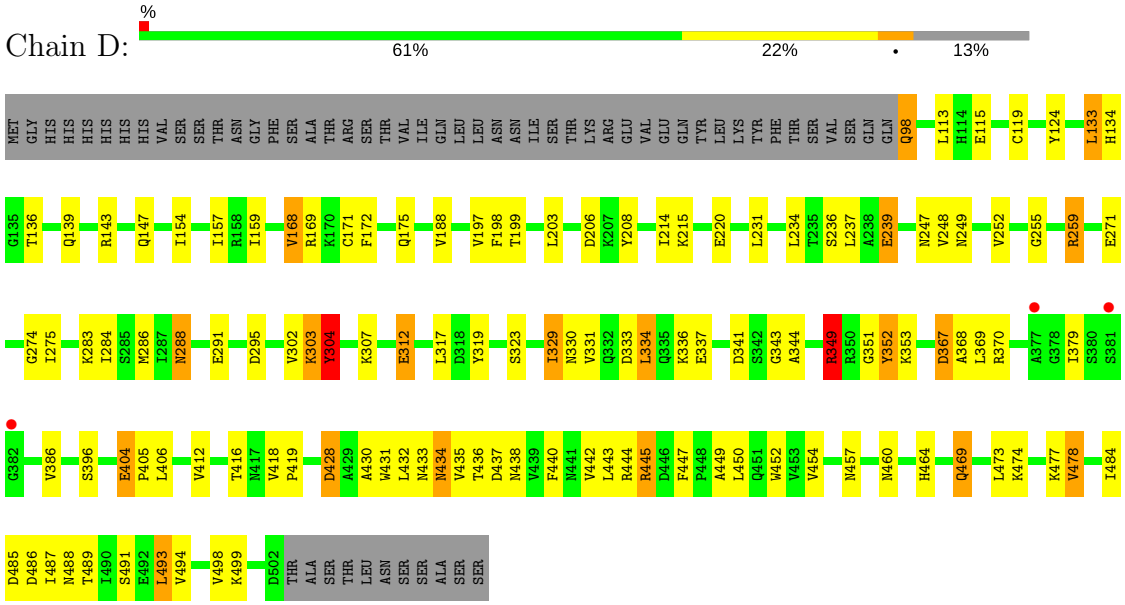
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain C:



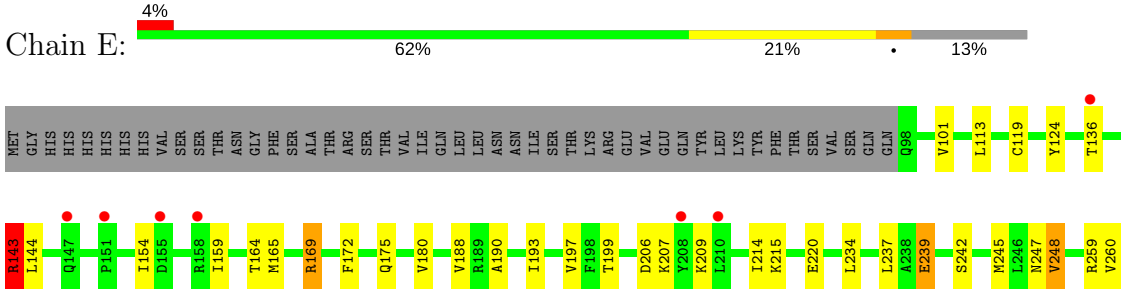
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

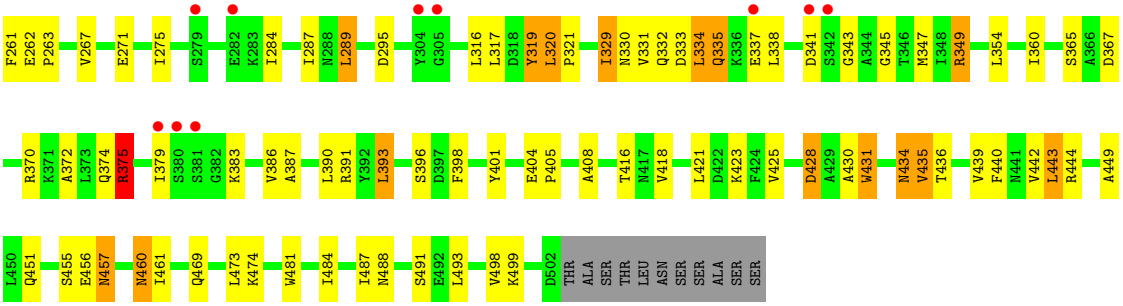
Chain D:



• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

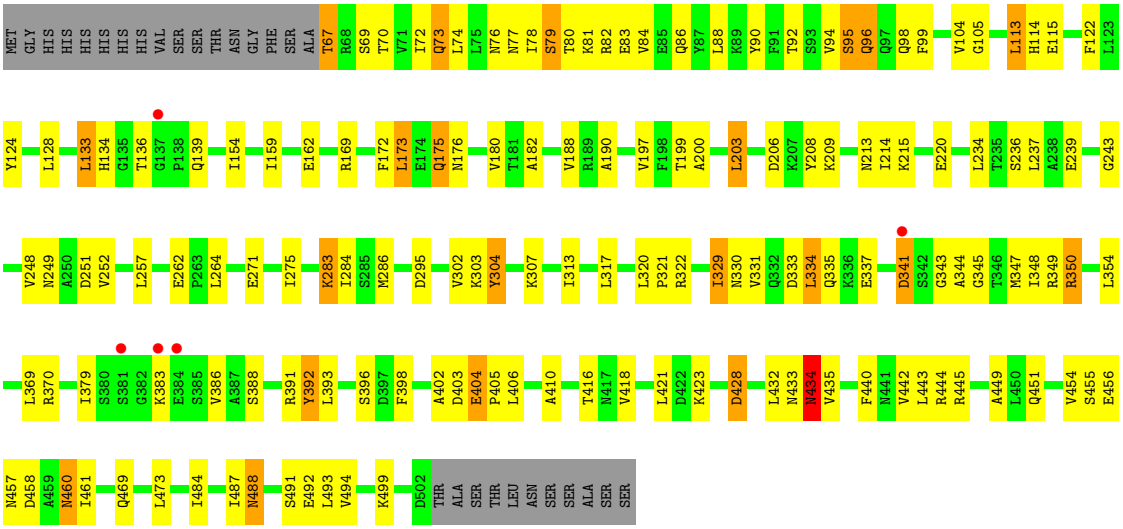
Chain E:





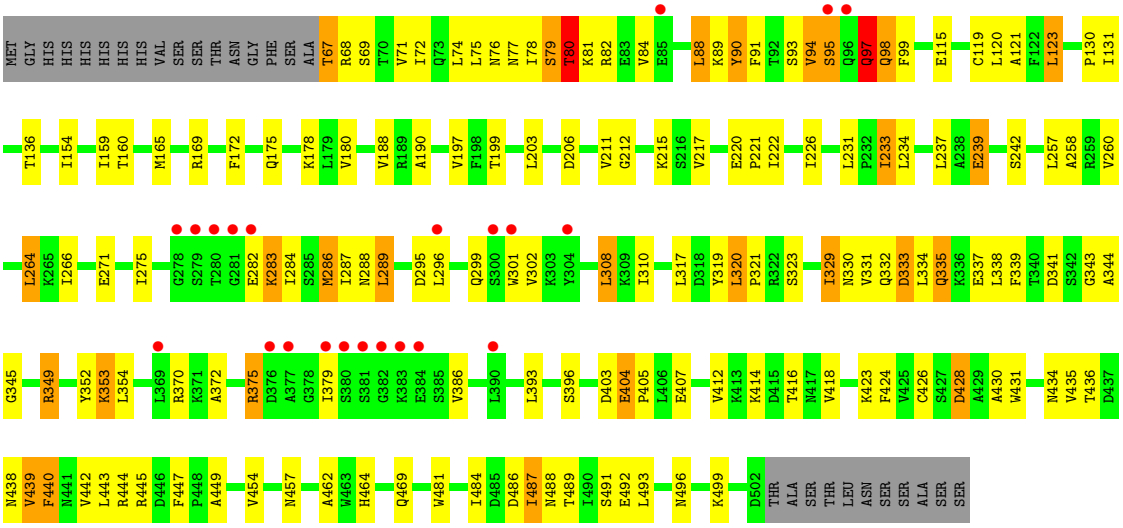
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain F:



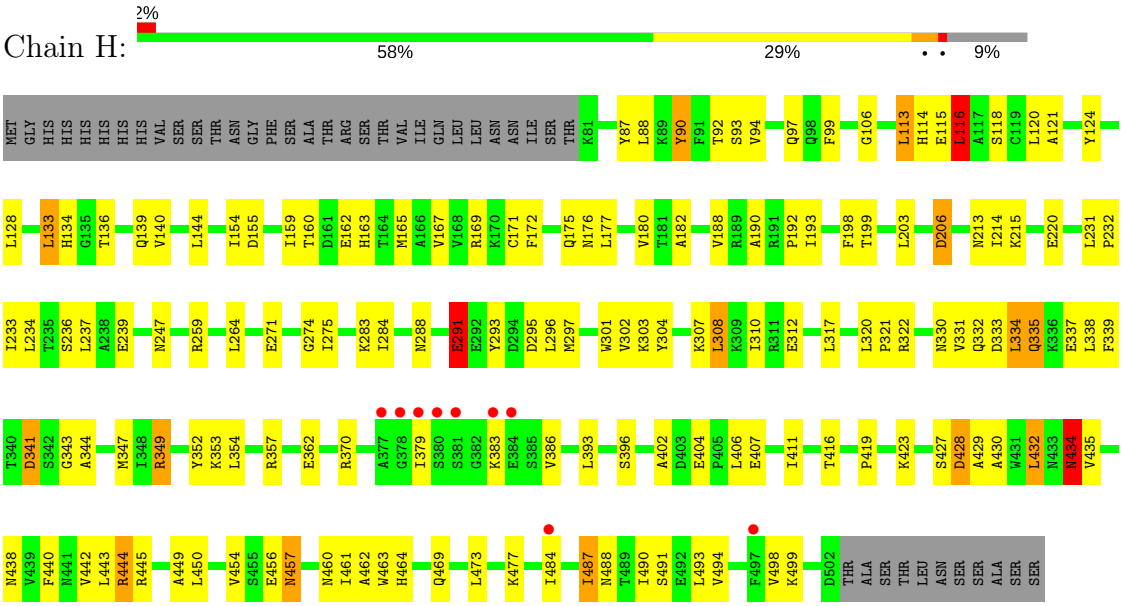
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain G:



• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain H:


2%
58%
29%
9%
MET GLY HIS HIS HIS HIS HIS VAL SER SER THR ASN GLY PHE SER ALA THR ARG SER THR VAL ILE GLN LEU LEU ASN ASN ILE SER THR K81 Y87 L88 K89 Y90 F91 T92 S93 V94 Q97 Q98 F99 G106 L113 H114 E115 L116 A117 S118 C119 L120 A121 Y124
L128 L133 H134 G135 T136 Q139 V140 L144 I154 D155 I159 T160 D161 E162 H163 T164 M165 A166 V167 V168 R169 K170 C171 F172 Q175 N176 L177 V180 T181 A182 V188 R189 A190 R191 P192 I193 F198 T199 L203 D206 N213 I214 K215 E220 L231 P232
I233 L234 T235 S236 L237 A238 E239 N247 R259 L264 E271 G274 I275 K283 I284 N288 E291 E292 Y293 D294 D295 L296 M297 W301 V302 K303 Y304 K307 L308 K309 I310 R311 E312 L317 L320 P321 R322 N330 V331 Q332 D333 L334 Q335 K336 E337 L338 F339
T340 D341 S342 G343 A344 M347 I348 R349 Y352 K353 L354 R357 E362 R370 A377 G378 I379 S380 S381 G382 K383 E384 S385 V386 L393 S396 A402 D403 E404 P405 L406 E407 I411 T416 P419 K423 S427 D428 A429 A430 W431 L432 N433 N434 V435
N438 V439 F440 N441 V442 L443 R444 R445 A449 L450 V454 S455 E456 N457 N460 I461 A462 W463 H464 Q469 L473 K477 I484 I487 N488 T489 I490 S491 E492 L493 V494 F497 V498 K499 D502 THR ALA SER THR LEU ASN SER SER ALA SER SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.88Å 103.27Å 111.31Å 77.31° 89.27° 70.43°	Depositor
Resolution (Å)	108.36 – 3.25 48.66 – 3.25	Depositor EDS
% Data completeness (in resolution range)	96.2 (108.36-3.25) 88.4 (48.66-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.193 , 0.238 0.196 , 0.240	Depositor DCC
R_{free} test set	2874 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	81.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	26320	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.75	1/3195 (0.0%)	0.90	6/4329 (0.1%)
1	B	0.80	2/3458 (0.1%)	0.96	10/4685 (0.2%)
1	C	0.78	4/3452 (0.1%)	0.94	8/4678 (0.2%)
1	D	0.75	2/3195 (0.1%)	0.94	5/4329 (0.1%)
1	E	0.71	2/3197 (0.1%)	0.89	8/4332 (0.2%)
1	F	0.76	1/3460 (0.0%)	0.93	9/4686 (0.2%)
1	G	0.74	3/3454 (0.1%)	0.99	13/4681 (0.3%)
1	H	0.75	3/3338 (0.1%)	0.92	8/4522 (0.2%)
All	All	0.76	18/26749 (0.1%)	0.93	67/36242 (0.2%)

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	B	0	2
1	C	0	1
1	F	0	2
1	G	0	1
All	All	0	6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	481	TRP	CD2-CE2	6.25	1.48	1.41
1	G	481	TRP	CD2-CE2	6.19	1.48	1.41
1	H	463	TRP	CD2-CE2	6.03	1.48	1.41
1	D	452	TRP	CD2-CE2	5.69	1.48	1.41
1	H	274	GLY	N-CA	-5.59	1.37	1.46
1	D	274	GLY	N-CA	-5.44	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	THR	N-CA	5.41	1.57	1.46
1	C	95	SER	CA-CB	5.40	1.61	1.52
1	A	481	TRP	CD2-CE2	5.37	1.47	1.41
1	G	404	GLU	CD-OE2	5.29	1.31	1.25
1	C	67	THR	N-CA	5.26	1.56	1.46
1	F	492	GLU	CD-OE2	5.22	1.31	1.25
1	B	282	GLU	CG-CD	5.21	1.59	1.51
1	C	301	TRP	CD2-CE2	5.17	1.47	1.41
1	H	301	TRP	CD2-CE2	5.07	1.47	1.41
1	E	431	TRP	CD2-CE2	5.04	1.47	1.41
1	G	301	TRP	CD2-CE2	5.03	1.47	1.41
1	C	481	TRP	CD2-CE2	5.01	1.47	1.41

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	375	ARG	NE-CZ-NH2	-21.70	109.45	120.30
1	G	375	ARG	NE-CZ-NH1	18.23	129.41	120.30
1	E	143	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	E	375	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	B	370	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	E	143	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	B	444	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	H	444	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	E	375	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	D	304	TYR	CB-CG-CD2	-8.06	116.17	121.00
1	C	319	TYR	CA-CB-CG	-7.51	99.13	113.40
1	H	349	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	423	LYS	CB-CG-CD	7.30	130.59	111.60
1	B	179	LEU	CB-CG-CD2	-7.22	98.72	111.00
1	F	350	ARG	CG-CD-NE	-7.19	96.70	111.80
1	G	90	TYR	CA-CB-CG	7.00	126.71	113.40
1	F	392	TYR	CB-CG-CD1	6.77	125.06	121.00
1	E	349	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	432	LEU	CA-CB-CG	6.54	130.33	115.30
1	D	259	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	322	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	237	LEU	CB-CG-CD1	-6.39	100.14	111.00
1	C	67	THR	N-CA-CB	6.35	122.37	110.30
1	H	291	GLU	CA-CB-CG	6.29	127.23	113.40
1	F	492	GLU	CG-CD-OE1	-6.23	105.84	118.30
1	B	296	LEU	CB-CG-CD1	-6.21	100.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	349	ARG	CG-CD-NE	6.20	124.83	111.80
1	D	304	TYR	CB-CG-CD1	6.17	124.70	121.00
1	A	444	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	393	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	F	492	GLU	CG-CD-OE2	5.97	130.23	118.30
1	G	264	LEU	CA-CB-CG	-5.80	101.97	115.30
1	B	393	LEU	CA-CB-CG	5.78	128.58	115.30
1	H	90	TYR	CA-CB-CG	5.70	124.22	113.40
1	H	259	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	E	319	TYR	CA-CB-CG	5.65	124.14	113.40
1	C	349	ARG	CB-CG-CD	-5.62	96.99	111.60
1	G	319	TYR	CA-CB-CG	5.62	124.08	113.40
1	A	308	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	G	123	LEU	CB-CG-CD2	-5.54	101.58	111.00
1	F	392	TYR	CB-CA-C	-5.54	99.33	110.40
1	E	169	ARG	CA-CB-CG	-5.51	101.28	113.40
1	B	370	ARG	CB-CG-CD	5.51	125.92	111.60
1	G	233	ILE	CG1-CB-CG2	-5.48	99.34	111.40
1	D	349	ARG	CG-CD-NE	-5.46	100.33	111.80
1	G	178	LYS	CD-CE-NZ	5.39	124.11	111.70
1	H	116	LEU	CA-CB-CG	5.39	127.70	115.30
1	G	80	THR	N-CA-C	-5.35	96.55	111.00
1	D	445	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	F	392	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	319	TYR	CA-CB-CG	-5.28	103.37	113.40
1	C	173	LEU	CA-CB-CG	5.25	127.38	115.30
1	G	353	LYS	N-CA-C	-5.24	96.84	111.00
1	B	444	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	H	206	ASP	CB-CG-OD1	5.23	123.00	118.30
1	B	370	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	G	203	LEU	CA-CB-CG	5.19	127.24	115.30
1	G	295	ASP	CB-CG-OD2	5.17	122.95	118.30
1	G	414	LYS	CD-CE-NZ	-5.13	99.90	111.70
1	F	304	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	F	264	LEU	CB-CG-CD1	-5.12	102.30	111.00
1	A	443	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	F	203	LEU	CA-CB-CG	5.09	127.01	115.30
1	H	128	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	B	257	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	C	334	LEU	CA-CB-CG	5.02	126.86	115.30
1	C	453	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	92	THR	Peptide
1	B	96	GLN	Peptide
1	C	95	SER	Peptide
1	F	95	SER	Peptide
1	F	96	GLN	Peptide
1	G	80	THR	Peptide

5.2 Too-close contacts (i)

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	3140	0	3153	101	1
1	B	3400	0	3418	135	0
1	C	3394	0	3407	129	1
1	D	3140	0	3153	116	0
1	E	3142	0	3153	107	1
1	F	3402	0	3429	151	1
1	G	3396	0	3407	153	1
1	H	3280	0	3286	100	1
2	D	13	0	9	10	0
2	H	13	0	9	2	0
All	All	26320	0	26424	916	3

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 17.

All (916) 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)
1:B:474:LYS:HE2	1:B:501:CYS:SG	1.27	1.67
1:B:474:LYS:CE	1:B:501:CYS:SG	2.09	1.38
1:F:72:ILE:O	1:G:89:LYS:NZ	1.65	1.29
1:B:379:ILE:HD11	1:B:423:LYS:NZ	1.52	1.23
1:B:379:ILE:HG21	1:B:386:VAL:CG2	1.72	1.20
1:E:379:ILE:HD11	1:E:423:LYS:NZ	1.56	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ILE:HG21	1:C:386:VAL:HG23	1.24	1.18
1:B:474:LYS:HD2	1:B:474:LYS:O	1.43	1.18
1:D:286:MET:HE1	1:D:438:ASN:ND2	1.60	1.15
1:D:352:TYR:OH	1:D:435:VAL:HG12	1.43	1.14
1:B:379:ILE:CG2	1:B:386:VAL:HG23	1.76	1.14
1:H:379:ILE:HD11	1:H:423:LYS:NZ	1.61	1.14
1:D:286:MET:HE1	1:D:438:ASN:HD21	0.97	1.12
1:A:387:ALA:HB2	1:E:262:GLU:OE2	1.50	1.10
1:G:379:ILE:HG21	1:G:386:VAL:HG23	1.24	1.10
1:F:379:ILE:HG21	1:F:386:VAL:HG23	1.17	1.09
1:F:94:VAL:HG21	1:G:68:ARG:NH2	1.68	1.09
1:F:379:ILE:HD11	1:F:423:LYS:HE3	1.35	1.08
1:F:249:ASN:HD22	1:F:252:VAL:HG23	1.21	1.06
1:G:77:ASN:O	1:G:81:LYS:NZ	1.88	1.05
1:F:80:THR:HG22	1:F:82:ARG:H	1.20	1.04
1:H:379:ILE:HD11	1:H:423:LYS:HZ3	1.22	1.03
1:B:283:LYS:HZ2	1:B:344:ALA:HA	1.23	1.01
1:D:98:GLN:HA	1:D:98:GLN:HE21	1.19	1.01
1:F:81:LYS:HE3	1:G:78:ILE:HG21	1.38	1.01
1:F:81:LYS:CE	1:G:78:ILE:HG21	1.91	1.00
1:F:249:ASN:ND2	1:F:252:VAL:HG23	1.76	1.00
1:B:379:ILE:HG21	1:B:386:VAL:HG23	1.01	1.00
1:D:249:ASN:N	2:D:1503:NLG:H8C3	1.77	0.99
1:E:370:ARG:HG3	1:E:386:VAL:HG11	1.44	0.98
1:E:379:ILE:HD11	1:E:423:LYS:HZ2	1.17	0.98
1:B:86:GLN:HG2	1:B:339:PHE:O	1.64	0.98
1:G:79:SER:OG	1:G:84:VAL:HG21	1.62	0.98
1:E:169:ARG:NE	1:E:245:MET:SD	2.37	0.97
1:D:352:TYR:OH	1:D:435:VAL:CG1	2.11	0.96
1:B:379:ILE:HD11	1:B:423:LYS:HZ3	1.16	0.96
1:H:379:ILE:HG21	1:H:386:VAL:HG23	1.47	0.96
1:C:276:ILE:CD1	1:C:283:LYS:HD2	1.96	0.96
1:C:453:VAL:HG12	1:C:453:VAL:O	1.66	0.95
1:E:379:ILE:HG21	1:E:386:VAL:HG23	1.47	0.95
1:B:379:ILE:HD11	1:B:423:LYS:HZ2	1.33	0.93
1:D:370:ARG:HG3	1:D:386:VAL:HG11	1.50	0.93
1:D:379:ILE:HG21	1:D:386:VAL:HG23	1.50	0.93
1:G:160:THR:HG21	1:G:165:MET:HE1	1.50	0.93
1:F:379:ILE:CG2	1:F:386:VAL:HG23	1.99	0.93
2:D:1503:NLG:CB	2:D:1503:NLG:H8C1	1.98	0.92
1:D:286:MET:CE	1:D:438:ASN:ND2	2.31	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:ILE:HD11	1:G:423:LYS:NZ	1.84	0.92
1:G:430:ALA:HB1	1:G:435:VAL:HG21	1.50	0.92
1:H:165:MET:HE1	1:H:247:ASN:HB2	1.50	0.91
1:B:474:LYS:HE2	1:B:501:CYS:HG	1.24	0.91
1:B:474:LYS:C	1:B:474:LYS:HD2	1.90	0.90
1:F:379:ILE:HG21	1:F:386:VAL:CG2	2.01	0.90
1:D:275:ILE:HG22	1:D:284:ILE:HD12	1.53	0.90
1:C:484:ILE:HD11	1:C:493:LEU:HD22	1.50	0.90
1:C:154:ILE:HG13	1:C:159:ILE:HD11	1.52	0.90
1:B:249:ASN:ND2	1:B:252:VAL:HG23	1.86	0.89
1:D:154:ILE:HG13	1:D:159:ILE:HD11	1.53	0.89
1:F:379:ILE:HD11	1:F:423:LYS:CE	2.03	0.88
1:E:143:ARG:HH11	1:E:143:ARG:HG3	1.38	0.88
1:F:80:THR:HG22	1:F:82:ARG:N	1.87	0.88
1:A:387:ALA:HB2	1:E:262:GLU:CD	1.94	0.88
1:D:430:ALA:HB1	1:D:435:VAL:HG21	1.56	0.88
1:C:379:ILE:CG2	1:C:386:VAL:HG23	2.04	0.87
1:A:370:ARG:HG2	1:A:386:VAL:HG11	1.55	0.87
1:F:90:TYR:HE2	1:F:128:LEU:HD11	1.36	0.87
1:A:387:ALA:CB	1:E:262:GLU:OE2	2.23	0.86
1:G:424:PHE:CZ	1:G:436:THR:HG22	2.10	0.86
1:D:214:ILE:HD11	1:D:248:VAL:HG11	1.58	0.86
1:A:136:THR:HG23	1:A:136:THR:O	1.73	0.86
1:H:133:LEU:HD21	1:H:236:SER:HB3	1.59	0.85
1:B:73:GLN:O	1:B:77:ASN:ND2	2.09	0.85
1:C:169:ARG:NH2	1:D:239:GLU:HG3	1.90	0.85
1:G:430:ALA:HB1	1:G:435:VAL:CG2	2.06	0.85
1:E:379:ILE:HD11	1:E:423:LYS:HZ3	1.38	0.84
1:F:81:LYS:HE3	1:G:78:ILE:CD1	2.08	0.84
1:D:323:SER:HA	1:D:433:ASN:HD21	1.41	0.84
1:D:98:GLN:HA	1:D:98:GLN:NE2	1.93	0.84
1:B:474:LYS:C	1:B:474:LYS:CD	2.46	0.84
1:C:379:ILE:HG21	1:C:386:VAL:CG2	2.05	0.84
1:E:154:ILE:HG13	1:E:159:ILE:HD11	1.59	0.84
1:H:180:VAL:HG13	1:H:190:ALA:HB3	1.60	0.84
1:G:197:VAL:HG21	1:G:234:LEU:HD11	1.58	0.84
1:A:404:GLU:OE2	1:E:365:SER:OG	1.95	0.83
1:B:283:LYS:NZ	1:B:344:ALA:HA	1.93	0.83
1:E:370:ARG:HG3	1:E:386:VAL:CG1	2.09	0.83
1:H:154:ILE:HG13	1:H:159:ILE:HD11	1.61	0.82
1:G:484:ILE:HD11	1:G:493:LEU:HD22	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:TRP:CZ3	1:D:436:THR:HG21	2.16	0.81
1:D:98:GLN:HE21	1:D:98:GLN:CA	1.93	0.81
1:B:154:ILE:HG13	1:B:159:ILE:HD11	1.63	0.81
1:G:449:ALA:HB1	1:G:484:ILE:HG23	1.62	0.81
1:G:80:THR:CG2	1:G:80:THR:O	2.29	0.80
1:H:379:ILE:HD11	1:H:423:LYS:HZ2	1.44	0.80
1:B:249:ASN:HD22	1:B:252:VAL:HG23	1.45	0.80
1:F:94:VAL:HG21	1:G:68:ARG:HH21	1.43	0.80
1:B:197:VAL:HG21	1:B:234:LEU:HD11	1.63	0.80
1:C:275:ILE:HG22	1:C:284:ILE:HD12	1.62	0.80
1:F:286:MET:HG3	1:F:434:ASN:HD22	1.47	0.80
1:F:133:LEU:HD21	1:F:236:SER:HB3	1.64	0.79
1:F:90:TYR:CE2	1:F:128:LEU:HD11	2.16	0.79
1:D:203:LEU:HD23	1:D:208:TYR:CD2	2.18	0.79
1:H:291:GLU:HG2	1:H:353:LYS:HE3	1.62	0.79
1:C:197:VAL:HG21	1:C:234:LEU:HD11	1.64	0.79
1:C:67:THR:HG21	1:C:69:SER:OG	1.83	0.79
1:C:276:ILE:HD13	1:C:283:LYS:HD2	1.65	0.78
1:C:94:VAL:HG11	1:C:98:GLN:OE1	1.83	0.78
1:D:430:ALA:HB1	1:D:435:VAL:CG2	2.14	0.77
1:B:275:ILE:HG22	1:B:284:ILE:HD12	1.66	0.77
1:G:424:PHE:HZ	1:G:436:THR:HG22	1.49	0.77
1:A:308:LEU:HD12	1:A:308:LEU:O	1.85	0.77
1:H:293:TYR:CE1	1:H:297:MET:HE2	2.19	0.77
1:D:133:LEU:HD21	1:D:236:SER:HB3	1.66	0.77
1:B:332:GLN:O	1:B:335:GLN:NE2	2.18	0.77
1:F:484:ILE:HD11	1:F:493:LEU:HD22	1.66	0.77
2:D:1503:NLG:HBC1	2:D:1503:NLG:H8C1	1.65	0.77
1:D:255:GLY:HA3	1:D:312:GLU:OE2	1.85	0.77
1:B:474:LYS:NZ	1:B:501:CYS:SG	2.57	0.77
1:F:283:LYS:HZ2	1:F:344:ALA:HA	1.48	0.77
1:F:81:LYS:HE3	1:G:78:ILE:HD12	1.66	0.76
1:F:73:GLN:NE2	1:F:335:GLN:HE21	1.84	0.75
1:A:260:VAL:HG12	1:A:261:PHE:CD2	2.22	0.75
1:C:369:LEU:HD22	1:C:373:LEU:HD11	1.68	0.75
1:F:81:LYS:CD	1:G:78:ILE:HG21	2.16	0.75
1:D:286:MET:CE	1:D:438:ASN:HD21	1.88	0.75
1:F:379:ILE:CD1	1:F:423:LYS:HE3	2.16	0.74
1:G:379:ILE:HD11	1:G:423:LYS:HZ2	1.50	0.74
1:B:180:VAL:HG13	1:B:190:ALA:HB3	1.67	0.74
1:C:73:GLN:O	1:C:77:ASN:ND2	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:THR:O	1:F:136:THR:HG23	1.87	0.74
1:G:286:MET:CE	1:G:288:ASN:OD1	2.35	0.74
1:F:88:LEU:HD21	1:G:76:ASN:HD21	1.53	0.74
1:A:144:LEU:HD23	1:A:167:VAL:HG21	1.69	0.74
1:C:453:VAL:CG1	1:C:453:VAL:O	2.33	0.73
1:D:370:ARG:HG3	1:D:386:VAL:CG1	2.17	0.73
1:E:317:LEU:HD23	1:E:320:LEU:HD12	1.68	0.73
1:H:322:ARG:NE	1:H:352:TYR:CZ	2.57	0.73
1:E:197:VAL:HG21	1:E:234:LEU:HD11	1.71	0.73
1:F:442:VAL:HG13	1:F:445:ARG:NH1	2.03	0.73
1:H:291:GLU:HG3	1:H:353:LYS:HG3	1.70	0.73
1:D:352:TYR:OH	1:D:435:VAL:CB	2.35	0.73
1:G:136:THR:HG23	1:G:136:THR:O	1.89	0.73
1:B:474:LYS:CD	1:B:474:LYS:O	2.31	0.73
1:C:276:ILE:CD1	1:C:283:LYS:CD	2.66	0.73
1:C:291:GLU:OE2	1:C:442:VAL:HG22	1.89	0.73
1:A:154:ILE:HG13	1:A:159:ILE:HD11	1.70	0.72
1:B:86:GLN:CG	1:B:339:PHE:O	2.36	0.72
1:C:136:THR:HG22	1:C:172:PHE:CE1	2.24	0.72
1:C:239:GLU:HG3	1:D:169:ARG:NH2	2.05	0.72
1:F:249:ASN:HD22	1:F:252:VAL:CG2	2.00	0.72
1:B:360:ILE:HD11	1:B:393:LEU:HD13	1.71	0.72
1:C:172:PHE:CE2	1:C:237:LEU:HD13	2.23	0.72
1:D:430:ALA:O	1:D:435:VAL:HG13	1.90	0.72
1:G:80:THR:HG22	1:G:80:THR:O	1.89	0.72
1:C:276:ILE:HD11	1:C:283:LYS:HD2	1.69	0.72
1:C:93:SER:OG	1:C:94:VAL:N	2.22	0.71
1:D:248:VAL:C	2:D:1503:NLG:H8C3	2.10	0.71
1:B:465:PHE:CE2	1:C:461:ILE:HD12	2.25	0.71
1:A:418:VAL:HG21	1:A:484:ILE:HD13	1.72	0.71
1:G:172:PHE:CE2	1:G:237:LEU:HD13	2.26	0.71
1:B:484:ILE:HD11	1:B:493:LEU:HD22	1.72	0.71
1:D:352:TYR:HH	1:D:435:VAL:HG12	1.55	0.71
1:E:239:GLU:HG3	1:F:169:ARG:NH2	2.06	0.71
1:F:90:TYR:HE2	1:F:128:LEU:CD1	2.04	0.71
1:G:379:ILE:CG2	1:G:386:VAL:HG23	2.14	0.70
1:C:94:VAL:HG21	1:C:98:GLN:OE1	1.91	0.70
1:E:430:ALA:HB1	1:E:435:VAL:CG2	2.22	0.70
1:B:172:PHE:CE2	1:B:237:LEU:HD13	2.25	0.70
1:F:172:PHE:CD2	1:F:237:LEU:HD13	2.26	0.70
1:F:484:ILE:HD11	1:F:493:LEU:CD2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:VAL:HG12	1:D:169:ARG:N	2.06	0.70
1:G:449:ALA:CB	1:G:484:ILE:HG23	2.20	0.70
1:E:172:PHE:CE2	1:E:237:LEU:HD13	2.26	0.70
1:G:154:ILE:HG13	1:G:159:ILE:HD11	1.73	0.69
1:A:484:ILE:HD11	1:A:493:LEU:HD22	1.74	0.69
1:F:154:ILE:HG13	1:F:159:ILE:HD11	1.74	0.69
1:B:123:LEU:HD21	1:B:338:LEU:HD13	1.75	0.69
1:D:288:ASN:ND2	1:D:351:GLY:HA3	2.08	0.69
1:G:82:ARG:HH22	1:G:462:ALA:HB3	1.56	0.69
1:F:329:ILE:HG22	1:F:345:GLY:HA3	1.75	0.69
1:C:67:THR:HG22	1:C:69:SER:H	1.58	0.69
1:E:370:ARG:CG	1:E:386:VAL:HG11	2.23	0.69
1:B:249:ASN:HD22	1:B:252:VAL:CG2	2.05	0.68
1:F:180:VAL:HG13	1:F:190:ALA:HB3	1.75	0.68
1:F:286:MET:HG3	1:F:434:ASN:ND2	2.07	0.68
1:A:387:ALA:HB2	1:E:262:GLU:CG	2.23	0.68
1:C:85:GLU:OE1	1:C:432:LEU:HD22	1.92	0.68
1:E:275:ILE:HG22	1:E:284:ILE:HD12	1.75	0.68
1:D:197:VAL:HG21	1:D:234:LEU:HD11	1.76	0.68
1:C:430:ALA:HB1	1:C:435:VAL:HG22	1.76	0.68
1:F:86:GLN:HG3	1:F:432:LEU:HD13	1.76	0.67
1:E:425:VAL:O	1:E:425:VAL:HG12	1.94	0.67
1:G:97:GLN:OE1	1:G:98:GLN:N	2.28	0.67
1:H:136:THR:HG22	1:H:172:PHE:CE1	2.29	0.67
1:D:275:ILE:CG2	1:D:284:ILE:HD12	2.23	0.67
1:D:139:GLN:HG2	1:D:175:GLN:OE1	1.95	0.67
1:E:484:ILE:HD11	1:E:493:LEU:CD2	2.24	0.67
1:G:431:TRP:CZ3	1:G:436:THR:HG21	2.30	0.67
1:C:154:ILE:CG1	1:C:159:ILE:HD11	2.25	0.67
1:C:67:THR:CG2	1:C:69:SER:OG	2.43	0.67
1:F:402:ALA:HB1	1:F:406:LEU:HD23	1.77	0.67
1:D:442:VAL:HG13	1:D:445:ARG:NH1	2.09	0.66
1:A:180:VAL:HG13	1:A:190:ALA:HB3	1.77	0.66
1:C:172:PHE:CD2	1:C:237:LEU:HD13	2.30	0.66
1:C:276:ILE:HD11	1:C:283:LYS:CD	2.24	0.66
1:E:172:PHE:CD2	1:E:237:LEU:HD13	2.30	0.66
1:G:74:LEU:C	1:G:74:LEU:HD23	2.15	0.66
1:C:430:ALA:HB1	1:C:435:VAL:CG2	2.26	0.66
1:D:418:VAL:HG21	1:D:484:ILE:HD13	1.77	0.66
1:G:379:ILE:HD11	1:G:423:LYS:HZ3	1.59	0.66
1:B:465:PHE:HE2	1:C:461:ILE:HD12	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LEU:HD21	1:C:326:VAL:HG23	1.78	0.66
1:F:173:LEU:N	1:F:173:LEU:HD23	2.10	0.66
1:F:88:LEU:HD21	1:G:76:ASN:ND2	2.10	0.66
1:A:283:LYS:HZ2	1:A:344:ALA:HA	1.59	0.66
1:D:147:GLN:HG2	1:G:321:PRO:HG3	1.78	0.66
1:E:124:TYR:CD2	1:E:188:VAL:HG22	2.31	0.66
1:H:172:PHE:CE2	1:H:237:LEU:HD13	2.31	0.65
1:E:260:VAL:HG12	1:E:261:PHE:CD2	2.32	0.65
1:F:283:LYS:NZ	1:F:344:ALA:HA	2.10	0.65
1:E:317:LEU:HD23	1:E:320:LEU:CD1	2.27	0.65
1:F:286:MET:CE	1:F:434:ASN:ND2	2.59	0.65
1:C:180:VAL:HG13	1:C:190:ALA:HB3	1.78	0.65
1:A:262:GLU:OE2	1:E:387:ALA:HB2	1.97	0.65
1:G:84:VAL:HG12	1:G:88:LEU:HD12	1.79	0.65
1:B:74:LEU:HD11	1:B:78:ILE:HD11	1.79	0.65
1:F:124:TYR:CG	1:F:188:VAL:HG13	2.31	0.64
1:H:335:GLN:H	1:H:335:GLN:HE21	1.44	0.64
1:F:449:ALA:HB1	1:F:484:ILE:HG23	1.80	0.64
1:G:286:MET:HE3	1:G:287:ILE:N	2.12	0.64
1:A:449:ALA:HB1	1:A:484:ILE:HG23	1.79	0.64
1:F:176:ASN:O	1:F:180:VAL:HG23	1.96	0.64
1:E:169:ARG:NH2	1:F:239:GLU:OE2	2.30	0.64
1:E:449:ALA:HB1	1:E:484:ILE:HG23	1.79	0.64
1:E:484:ILE:HD11	1:E:493:LEU:HD22	1.80	0.64
1:G:239:GLU:HG3	1:H:169:ARG:NH2	2.13	0.64
1:H:484:ILE:HD11	1:H:493:LEU:HD22	1.79	0.64
1:F:180:VAL:HG13	1:F:190:ALA:CB	2.28	0.64
1:B:283:LYS:HZ2	1:B:344:ALA:CA	2.07	0.64
1:H:203:LEU:HD13	1:H:213:ASN:HD22	1.63	0.63
1:A:169:ARG:NH2	1:B:239:GLU:OE2	2.32	0.63
1:A:239:GLU:HG3	1:B:169:ARG:HH22	1.63	0.63
1:F:70:THR:HG23	1:F:122:PHE:CD1	2.34	0.63
1:E:136:THR:HG23	1:E:136:THR:O	1.99	0.63
1:D:248:VAL:C	2:D:1503:NLG:C8	2.66	0.63
1:C:147:GLN:HE22	1:C:167:VAL:HG22	1.63	0.63
1:E:379:ILE:CD1	1:E:423:LYS:HZ2	2.04	0.62
1:B:329:ILE:HG22	1:B:345:GLY:HA3	1.81	0.62
1:F:81:LYS:HG3	1:G:78:ILE:CG2	2.30	0.62
1:B:488:ASN:C	1:B:488:ASN:HD22	2.03	0.62
1:C:275:ILE:CG2	1:C:284:ILE:HD12	2.28	0.62
1:A:330:ASN:OD1	1:A:331:VAL:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:172:PHE:CD2	1:H:237:LEU:HD13	2.35	0.62
1:H:308:LEU:O	1:H:308:LEU:HD12	1.98	0.62
1:C:99:PHE:CZ	1:C:338:LEU:HD13	2.35	0.62
1:G:286:MET:HE2	1:G:288:ASN:OD1	1.99	0.62
1:H:293:TYR:HE1	1:H:297:MET:HE2	1.61	0.62
1:F:286:MET:CG	1:F:434:ASN:ND2	2.63	0.62
1:H:432:LEU:HD23	1:H:432:LEU:N	2.15	0.62
1:A:197:VAL:HG21	1:A:234:LEU:HD11	1.80	0.61
1:A:172:PHE:CE2	1:A:237:LEU:HD13	2.34	0.61
1:B:77:ASN:OD1	1:B:335:GLN:OE1	2.18	0.61
1:C:297:MET:HE2	1:C:297:MET:HA	1.82	0.61
1:F:84:VAL:HG13	1:G:75:LEU:HD22	1.81	0.61
1:E:144:LEU:HD11	1:E:164:THR:HG23	1.83	0.61
1:A:260:VAL:HG12	1:A:261:PHE:N	2.14	0.61
1:H:430:ALA:HB1	1:H:435:VAL:CG2	2.30	0.61
1:G:180:VAL:HG13	1:G:190:ALA:HB3	1.83	0.61
1:G:172:PHE:CD2	1:G:237:LEU:HD13	2.35	0.61
1:G:431:TRP:CH2	1:G:436:THR:HG21	2.36	0.61
1:B:368:ALA:HB1	1:B:406:LEU:HD13	1.81	0.61
1:G:120:LEU:HA	1:G:123:LEU:HD12	1.83	0.61
1:G:430:ALA:O	1:G:435:VAL:HG13	2.00	0.61
1:A:124:TYR:CG	1:A:188:VAL:HG13	2.36	0.60
1:B:136:THR:HG23	1:B:136:THR:O	2.01	0.60
1:A:386:VAL:HG12	1:A:387:ALA:N	2.15	0.60
1:B:341:ASP:HA	1:B:347:MET:HE1	1.82	0.60
1:F:74:LEU:HD21	1:F:78:ILE:HD11	1.83	0.60
1:B:283:LYS:NZ	1:B:344:ALA:CA	2.63	0.60
1:H:442:VAL:HG13	1:H:445:ARG:NH1	2.15	0.60
2:D:1503:NLG:HBC2	2:D:1503:NLG:H8C1	1.82	0.60
1:G:286:MET:HE1	1:G:288:ASN:OD1	2.01	0.60
1:H:275:ILE:HG22	1:H:284:ILE:HD12	1.83	0.60
1:B:317:LEU:HD21	1:B:326:VAL:HG23	1.84	0.60
1:D:323:SER:HA	1:D:433:ASN:ND2	2.15	0.60
1:E:317:LEU:HA	1:E:320:LEU:HD12	1.84	0.60
1:G:169:ARG:NH2	1:H:239:GLU:HG3	2.17	0.60
1:H:291:GLU:CG	1:H:353:LYS:HG3	2.32	0.60
1:C:94:VAL:HG13	1:H:163:HIS:CD2	2.37	0.59
1:D:172:PHE:CE2	1:D:237:LEU:HD13	2.36	0.59
1:C:330:ASN:OD1	1:C:331:VAL:N	2.35	0.59
1:E:267:VAL:HG21	1:E:338:LEU:HD21	1.83	0.59
1:H:288:ASN:ND2	1:H:438:ASN:HD21	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:LYS:CD	1:B:501:CYS:SG	2.89	0.59
1:E:430:ALA:HB1	1:E:435:VAL:HG21	1.84	0.59
1:H:341:ASP:OD2	1:H:432:LEU:HD12	2.03	0.59
1:F:484:ILE:CD1	1:F:493:LEU:HD22	2.31	0.59
1:C:165:MET:HE1	1:C:247:ASN:HB2	1.84	0.59
1:H:302:VAL:HG12	1:H:307:LYS:HG3	1.83	0.59
1:H:393:LEU:HD11	1:H:411:ILE:HD13	1.85	0.59
1:F:74:LEU:CD2	1:F:78:ILE:HD11	2.33	0.59
1:E:430:ALA:HB1	1:E:435:VAL:HG22	1.85	0.59
1:D:418:VAL:CG2	1:D:484:ILE:HD13	2.32	0.58
1:F:442:VAL:HG13	1:F:445:ARG:HH12	1.69	0.58
1:B:172:PHE:CD2	1:B:237:LEU:HD13	2.37	0.58
1:C:297:MET:CE	1:C:297:MET:HA	2.33	0.58
1:D:124:TYR:CG	1:D:188:VAL:HG13	2.37	0.58
1:E:154:ILE:CG1	1:E:159:ILE:HD11	2.33	0.58
1:B:77:ASN:HB3	1:B:336:LYS:HG3	1.86	0.58
1:E:474:LYS:HD3	1:E:498:VAL:HG22	1.86	0.58
1:G:330:ASN:OD1	1:G:331:VAL:N	2.36	0.58
1:B:379:ILE:HD13	1:B:386:VAL:HG22	1.85	0.58
1:C:369:LEU:HD22	1:C:373:LEU:CD1	2.33	0.58
1:F:94:VAL:HG21	1:G:68:ARG:CZ	2.31	0.58
1:D:136:THR:HG22	1:D:172:PHE:CE1	2.38	0.58
1:C:449:ALA:HB1	1:C:484:ILE:HG23	1.85	0.58
1:E:237:LEU:HD23	1:E:245:MET:CE	2.33	0.58
1:F:302:VAL:HG12	1:F:307:LYS:HG3	1.86	0.58
1:F:80:THR:CG2	1:F:82:ARG:H	2.05	0.58
1:D:431:TRP:CH2	1:D:436:THR:HG21	2.39	0.57
1:A:442:VAL:HG13	1:A:445:ARG:NH1	2.18	0.57
1:F:133:LEU:HD23	1:F:134:HIS:N	2.18	0.57
1:G:119:CYS:SG	1:G:334:LEU:HD13	2.44	0.57
1:F:72:ILE:C	1:G:89:LYS:NZ	2.53	0.57
1:B:83:GLU:HB3	1:B:340:THR:HG22	1.86	0.57
1:F:94:VAL:HG12	1:F:94:VAL:O	2.04	0.57
1:C:124:TYR:CG	1:C:188:VAL:HG13	2.39	0.57
1:D:330:ASN:OD1	1:D:331:VAL:N	2.36	0.57
1:H:330:ASN:OD1	1:H:331:VAL:N	2.37	0.57
1:C:370:ARG:HG3	1:C:386:VAL:HG11	1.85	0.57
1:D:343:GLY:O	1:D:344:ALA:HB2	2.04	0.57
1:E:330:ASN:OD1	1:E:331:VAL:N	2.37	0.57
1:F:173:LEU:N	1:F:173:LEU:CD2	2.68	0.57
1:F:79:SER:HA	1:G:82:ARG:HD3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:ILE:HG22	1:E:345:GLY:HA3	1.86	0.57
1:G:308:LEU:O	1:G:308:LEU:HD12	2.04	0.57
1:D:198:PHE:CD1	1:D:214:ILE:HD13	2.40	0.57
1:D:419:PRO:O	1:D:450:LEU:HD12	2.04	0.57
1:E:484:ILE:CD1	1:E:493:LEU:HD22	2.35	0.57
1:C:97:GLN:NE2	1:C:223:GLU:OE2	2.38	0.57
1:H:332:GLN:O	1:H:335:GLN:NE2	2.38	0.57
1:B:275:ILE:CG2	1:B:284:ILE:HD12	2.34	0.57
1:B:330:ASN:OD1	1:B:331:VAL:N	2.38	0.57
1:G:95:SER:HB3	1:G:98:GLN:HB2	1.87	0.57
1:A:317:LEU:HA	1:A:320:LEU:HD12	1.87	0.56
1:H:198:PHE:CD1	1:H:214:ILE:HD13	2.39	0.56
1:A:144:LEU:HD11	1:A:164:THR:HG23	1.88	0.56
1:C:249:ASN:HB3	1:C:252:VAL:HG23	1.86	0.56
1:F:124:TYR:CD2	1:F:188:VAL:HG13	2.40	0.56
1:D:124:TYR:CD2	1:D:188:VAL:HG13	2.40	0.56
1:D:431:TRP:CE3	1:D:436:THR:HG21	2.40	0.56
1:F:77:ASN:HD22	1:F:77:ASN:N	2.03	0.56
1:F:330:ASN:OD1	1:F:331:VAL:N	2.39	0.56
1:H:293:TYR:CE1	1:H:297:MET:CE	2.89	0.56
1:F:418:VAL:HG21	1:F:484:ILE:HD13	1.87	0.56
1:F:98:GLN:NE2	1:F:99:PHE:H	2.04	0.56
1:B:136:THR:HG22	1:B:172:PHE:CE1	2.41	0.56
1:F:81:LYS:CE	1:G:78:ILE:HD12	2.34	0.56
1:G:97:GLN:C	1:G:99:PHE:H	2.09	0.56
1:G:333:ASP:N	1:G:333:ASP:OD1	2.39	0.56
1:C:424:PHE:HE1	1:C:439:VAL:HG11	1.70	0.56
1:F:197:VAL:HG21	1:F:234:LEU:HD11	1.87	0.56
1:F:77:ASN:ND2	1:F:77:ASN:N	2.53	0.56
1:A:332:GLN:O	1:A:335:GLN:NE2	2.35	0.55
1:B:133:LEU:HD23	1:B:254:ALA:HA	1.87	0.55
1:C:128:LEU:HD12	1:C:339:PHE:HZ	1.70	0.55
1:D:139:GLN:CD	1:D:139:GLN:H	2.10	0.55
1:F:73:GLN:HE22	1:F:335:GLN:HE21	1.54	0.55
1:A:119:CYS:SG	1:A:334:LEU:HD13	2.46	0.55
1:C:124:TYR:CD2	1:C:188:VAL:HG13	2.41	0.55
1:C:379:ILE:HD11	1:C:423:LYS:NZ	2.21	0.55
1:D:286:MET:HG3	1:D:437:ASP:HB3	1.88	0.55
1:H:449:ALA:HB1	1:H:484:ILE:HG23	1.88	0.55
1:B:412:VAL:HG11	1:B:447:PHE:CE1	2.42	0.55
1:E:418:VAL:HG21	1:E:484:ILE:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:VAL:HG11	1:D:493:LEU:HD11	1.89	0.55
1:A:136:THR:O	1:A:136:THR:CG2	2.49	0.55
1:D:154:ILE:CG1	1:D:159:ILE:HD11	2.31	0.55
1:F:81:LYS:HE3	1:G:78:ILE:HD13	1.86	0.55
1:G:79:SER:OG	1:G:84:VAL:CG2	2.47	0.55
1:B:169:ARG:HH11	1:B:245:MET:HE1	1.72	0.55
1:D:352:TYR:N	1:D:352:TYR:CD1	2.73	0.55
1:G:283:LYS:HZ2	1:G:344:ALA:HA	1.72	0.55
1:H:487:ILE:HA	1:H:490:ILE:HD12	1.88	0.55
1:A:176:ASN:O	1:A:180:VAL:HG23	2.07	0.54
1:G:242:SER:HB3	1:H:162:GLU:HG2	1.89	0.54
1:H:180:VAL:HG13	1:H:190:ALA:CB	2.35	0.54
1:A:239:GLU:HG3	1:B:169:ARG:HH12	1.72	0.54
1:C:370:ARG:HG3	1:C:386:VAL:CG1	2.37	0.54
1:G:77:ASN:O	1:G:81:LYS:CE	2.54	0.54
1:A:418:VAL:CG2	1:A:484:ILE:HD13	2.38	0.54
1:A:283:LYS:NZ	1:A:344:ALA:HA	2.22	0.54
1:B:123:LEU:HD23	1:B:339:PHE:HZ	1.72	0.54
1:E:401:TYR:CE2	1:E:442:VAL:HG11	2.43	0.54
1:A:98:GLN:NE2	1:A:99:PHE:H	2.05	0.54
1:C:329:ILE:HG22	1:C:345:GLY:HA3	1.89	0.54
1:C:87:TYR:CE1	1:C:339:PHE:CD2	2.96	0.54
1:H:494:VAL:O	1:H:498:VAL:HG23	2.07	0.54
1:F:73:GLN:NE2	1:F:335:GLN:NE2	2.56	0.54
1:H:116:LEU:HD21	1:H:120:LEU:HD11	1.89	0.54
1:B:259:ARG:HG2	1:B:319:TYR:CE1	2.43	0.54
1:F:81:LYS:HG3	1:G:78:ILE:HG21	1.90	0.54
1:B:479:LEU:HD12	1:B:480:PHE:N	2.22	0.54
1:E:372:ALA:O	1:E:375:ARG:HD2	2.09	0.54
1:F:172:PHE:CD2	1:F:237:LEU:CD1	2.91	0.54
1:F:286:MET:HE1	1:F:434:ASN:ND2	2.23	0.54
1:H:430:ALA:HB1	1:H:435:VAL:HG22	1.88	0.54
1:A:444:ARG:HH11	1:A:444:ARG:CG	2.21	0.53
1:B:379:ILE:CD1	1:B:423:LYS:HZ2	2.14	0.53
1:C:128:LEU:HD12	1:C:339:PHE:CZ	2.42	0.53
1:D:172:PHE:CD2	1:D:237:LEU:HD13	2.43	0.53
1:G:84:VAL:HG12	1:G:88:LEU:CD1	2.38	0.53
1:H:335:GLN:H	1:H:335:GLN:NE2	2.05	0.53
1:A:249:ASN:ND2	1:A:252:VAL:HG23	2.23	0.53
1:D:286:MET:CE	1:D:438:ASN:HD22	2.20	0.53
1:A:172:PHE:CD2	1:A:237:LEU:HD13	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:TYR:OH	1:D:485:ASP:HB2	2.09	0.53
1:F:133:LEU:CD2	1:F:133:LEU:C	2.77	0.53
1:G:353:LYS:O	1:G:354:LEU:HD23	2.08	0.53
1:B:248:VAL:O	1:B:248:VAL:HG12	2.08	0.53
1:E:332:GLN:O	1:E:335:GLN:NE2	2.35	0.53
1:A:354:LEU:HD13	1:A:439:VAL:HG22	1.90	0.53
1:D:291:GLU:HG2	1:D:353:LYS:HA	1.91	0.53
1:C:428:ASP:N	1:C:428:ASP:OD1	2.42	0.53
1:D:368:ALA:HB1	1:D:406:LEU:HD13	1.91	0.53
1:G:93:SER:O	1:G:94:VAL:HG23	2.09	0.53
1:C:232:PRO:O	1:C:233:ILE:HD13	2.08	0.52
1:D:336:LYS:CD	1:D:343:GLY:HA2	2.38	0.52
1:B:379:ILE:CD1	1:B:423:LYS:HZ3	2.05	0.52
1:D:133:LEU:HD23	1:D:134:HIS:N	2.23	0.52
1:E:165:MET:HE1	1:E:247:ASN:HB2	1.90	0.52
1:B:154:ILE:CG1	1:B:159:ILE:HD11	2.38	0.52
1:D:449:ALA:HB1	1:D:484:ILE:HG23	1.91	0.52
1:D:147:GLN:HA	1:G:321:PRO:HB3	1.90	0.52
1:B:299:GLN:O	1:B:302:VAL:HG12	2.09	0.52
1:B:208:TYR:HB3	1:B:211:VAL:CG2	2.39	0.52
1:C:484:ILE:HD11	1:C:493:LEU:CD2	2.32	0.52
1:E:393:LEU:HD22	1:E:398:PHE:CD2	2.45	0.52
1:D:302:VAL:HG12	1:D:307:LYS:HG3	1.91	0.52
1:H:133:LEU:HD23	1:H:134:HIS:N	2.24	0.52
1:H:291:GLU:HG2	1:H:353:LYS:CE	2.36	0.52
1:C:442:VAL:HG13	1:C:445:ARG:NH1	2.25	0.52
1:F:113:LEU:HD11	1:F:182:ALA:HB2	1.92	0.52
1:B:87:TYR:CE2	1:B:339:PHE:CD2	2.98	0.52
1:D:136:THR:HG23	1:D:136:THR:O	2.10	0.52
1:E:379:ILE:CG2	1:E:386:VAL:HG23	2.33	0.52
1:F:81:LYS:CG	1:G:78:ILE:HG21	2.39	0.52
1:C:172:PHE:CE2	1:C:237:LEU:CD1	2.93	0.52
1:E:428:ASP:OD1	1:E:428:ASP:N	2.42	0.52
1:F:449:ALA:CB	1:F:484:ILE:HG23	2.38	0.52
1:H:116:LEU:CD2	1:H:120:LEU:HD11	2.40	0.52
1:B:144:LEU:CD2	1:B:167:VAL:HG21	2.41	0.51
1:C:198:PHE:CD1	1:C:214:ILE:HD13	2.46	0.51
1:E:180:VAL:HG13	1:E:190:ALA:HB3	1.92	0.51
1:G:84:VAL:O	1:G:88:LEU:HD12	2.10	0.51
1:G:221:PRO:HA	1:H:177:LEU:HD21	1.92	0.51
1:C:267:VAL:CG2	1:C:338:LEU:HD21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:154:ILE:CG1	1:H:159:ILE:HD11	2.35	0.51
1:E:119:CYS:SG	1:E:334:LEU:HD13	2.51	0.51
1:A:404:GLU:CD	1:E:365:SER:OG	2.49	0.51
1:G:74:LEU:O	1:G:77:ASN:HB2	2.10	0.51
1:H:136:THR:H	2:H:1503:NLG:HGC2	1.75	0.51
1:H:99:PHE:HZ	1:H:338:LEU:HD13	1.76	0.51
1:A:486:ASP:OD2	1:A:489:THR:HG23	2.11	0.51
1:D:428:ASP:OD1	1:D:428:ASP:N	2.43	0.51
1:B:291:GLU:HG2	1:B:353:LYS:HA	1.93	0.51
1:E:169:ARG:NH1	1:F:239:GLU:OE2	2.44	0.51
1:A:484:ILE:HD11	1:A:493:LEU:CD2	2.41	0.51
1:G:94:VAL:HG12	1:G:94:VAL:O	2.10	0.51
1:H:193:ILE:HB	1:H:234:LEU:HD13	1.92	0.51
1:A:162:GLU:HG2	1:B:242:SER:HB3	1.93	0.51
1:B:360:ILE:HD11	1:B:393:LEU:CD1	2.40	0.50
1:C:478:VAL:HG11	1:C:480:PHE:CZ	2.45	0.50
1:D:147:GLN:HA	1:G:321:PRO:CG	2.40	0.50
1:E:136:THR:HG22	1:E:172:PHE:CE1	2.47	0.50
1:F:74:LEU:HD13	1:G:71:VAL:HG13	1.92	0.50
1:A:428:ASP:OD1	1:A:428:ASP:N	2.42	0.50
1:D:317:LEU:HD13	1:D:349:ARG:HA	1.92	0.50
1:D:352:TYR:OH	1:D:435:VAL:HB	2.10	0.50
1:H:133:LEU:C	1:H:133:LEU:CD2	2.80	0.50
1:A:239:GLU:CG	1:B:169:ARG:HH12	2.24	0.50
1:C:393:LEU:HD11	1:C:411:ILE:HD13	1.92	0.50
1:F:329:ILE:HG21	1:F:337:GLU:HG3	1.93	0.50
1:D:147:GLN:HA	1:G:321:PRO:HG3	1.93	0.50
1:G:283:LYS:NZ	1:G:344:ALA:HA	2.26	0.50
1:D:336:LYS:HD2	1:D:343:GLY:HA2	1.94	0.50
1:H:427:SER:O	1:H:430:ALA:HB3	2.12	0.50
1:F:81:LYS:HE3	1:G:78:ILE:CG2	2.26	0.50
1:A:387:ALA:CA	1:E:262:GLU:OE2	2.59	0.49
1:F:275:ILE:HG22	1:F:284:ILE:HD12	1.93	0.49
1:F:86:GLN:CG	1:F:432:LEU:HD13	2.41	0.49
1:H:116:LEU:CD2	1:H:120:LEU:CD1	2.90	0.49
1:E:408:ALA:HB2	1:E:435:VAL:HG21	1.94	0.49
1:F:133:LEU:HD23	1:F:133:LEU:C	2.32	0.49
1:B:428:ASP:OD1	1:B:428:ASP:N	2.44	0.49
1:F:214:ILE:HD11	1:F:248:VAL:HG11	1.94	0.49
1:F:262:GLU:HA	1:F:320:LEU:HD22	1.93	0.49
1:G:97:GLN:HG2	1:G:226:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:CG1	1:A:261:PHE:N	2.75	0.49
1:F:456:GLU:OE2	1:F:473:LEU:HD21	2.11	0.49
1:C:367:ASP:HA	1:C:370:ARG:NH1	2.28	0.49
1:E:372:ALA:O	1:E:375:ARG:CD	2.61	0.49
1:F:388:SER:HB2	1:F:391:ARG:NH2	2.27	0.49
1:H:434:ASN:N	1:H:434:ASN:OD1	2.45	0.49
1:B:208:TYR:HB3	1:B:211:VAL:HG21	1.94	0.49
1:B:393:LEU:HD22	1:B:398:PHE:CE2	2.48	0.49
1:F:410:ALA:HB1	1:F:421:LEU:HD11	1.94	0.49
1:G:428:ASP:OD1	1:G:428:ASP:N	2.43	0.49
1:A:239:GLU:OE1	1:A:245:MET:HE3	2.13	0.49
1:A:329:ILE:HG22	1:A:345:GLY:HA3	1.93	0.49
1:B:486:ASP:OD2	1:B:489:THR:HG23	2.13	0.49
1:D:247:ASN:CG	2:D:1503:NLG:H8C2	2.33	0.49
1:G:90:TYR:OH	1:G:323:SER:HB2	2.13	0.49
1:A:154:ILE:CG1	1:A:159:ILE:HD11	2.41	0.49
1:A:275:ILE:HD12	1:A:346:THR:HG21	1.93	0.49
1:A:391:ARG:CB	1:E:319:TYR:HE2	2.25	0.49
1:B:180:VAL:HG13	1:B:190:ALA:CB	2.42	0.49
1:E:143:ARG:NH1	1:E:143:ARG:HG3	2.13	0.49
1:G:442:VAL:HG13	1:G:445:ARG:NH1	2.28	0.49
1:A:412:VAL:HG11	1:A:447:PHE:CE2	2.47	0.48
1:B:393:LEU:HD22	1:B:398:PHE:CD2	2.48	0.48
1:B:401:TYR:CE2	1:B:442:VAL:HG11	2.48	0.48
1:C:106:GLY:C	1:C:139:GLN:HE22	2.16	0.48
1:E:360:ILE:HD11	1:E:393:LEU:HD13	1.95	0.48
1:G:352:TYR:CE1	1:G:435:VAL:HG12	2.48	0.48
1:B:78:ILE:HA	1:B:83:GLU:OE1	2.12	0.48
1:D:418:VAL:HG22	1:D:484:ILE:HG21	1.93	0.48
1:E:418:VAL:CG2	1:E:484:ILE:HD13	2.44	0.48
1:G:296:LEU:CD2	1:G:310:ILE:HD13	2.43	0.48
1:C:434:ASN:N	1:C:434:ASN:OD1	2.46	0.48
1:A:387:ALA:HB1	1:E:259:ARG:O	2.13	0.48
1:E:418:VAL:HG11	1:E:493:LEU:HD21	1.95	0.48
1:F:418:VAL:CG2	1:F:484:ILE:HD13	2.43	0.48
1:F:88:LEU:HD11	1:G:76:ASN:HD22	1.77	0.48
1:H:457:ASN:C	1:H:457:ASN:HD22	2.16	0.48
1:G:97:GLN:HA	1:G:226:ILE:HD13	1.95	0.48
1:C:332:GLN:O	1:C:335:GLN:NE2	2.38	0.48
1:D:247:ASN:OD1	2:D:1503:NLG:H8C2	2.13	0.48
1:H:334:LEU:C	1:H:334:LEU:CD2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:LEU:O	1:B:203:LEU:HD12	2.14	0.48
1:B:449:ALA:HB1	1:B:484:ILE:HG23	1.96	0.48
1:F:78:ILE:HA	1:F:83:GLU:OE1	2.14	0.48
1:F:92:THR:HG23	1:G:72:ILE:HD13	1.95	0.48
2:H:1503:NLG:HGC1	2:H:1503:NLG:OXT	2.13	0.48
1:H:90:TYR:OH	1:H:264:LEU:HD22	2.14	0.48
1:B:316:LEU:O	1:B:316:LEU:HD12	2.14	0.48
1:F:393:LEU:HD22	1:F:398:PHE:CD2	2.47	0.48
1:F:434:ASN:N	1:F:434:ASN:OD1	2.47	0.48
1:B:123:LEU:HD21	1:B:338:LEU:CD1	2.42	0.48
1:F:286:MET:SD	1:F:434:ASN:ND2	2.87	0.48
1:G:484:ILE:HD11	1:G:493:LEU:CD2	2.38	0.48
1:G:492:GLU:O	1:G:496:ASN:ND2	2.47	0.48
1:B:119:CYS:SG	1:B:334:LEU:HD13	2.54	0.48
1:E:169:ARG:CZ	1:E:245:MET:SD	3.02	0.48
1:F:76:ASN:ND2	1:G:89:LYS:CE	2.77	0.48
1:C:136:THR:HG22	1:C:172:PHE:CZ	2.49	0.47
1:D:430:ALA:HA	1:D:435:VAL:CG1	2.43	0.47
1:E:237:LEU:HD23	1:E:245:MET:HE1	1.94	0.47
1:H:176:ASN:HD21	1:H:192:PRO:CB	2.27	0.47
1:A:313:ILE:HG23	1:A:326:VAL:HG21	1.95	0.47
1:E:214:ILE:HD11	1:E:248:VAL:HG11	1.96	0.47
1:F:334:LEU:C	1:F:334:LEU:CD2	2.83	0.47
1:G:275:ILE:HG22	1:G:284:ILE:HD12	1.96	0.47
1:D:249:ASN:N	2:D:1503:NLG:C8	2.62	0.47
1:G:418:VAL:HB	1:G:493:LEU:HD11	1.95	0.47
1:F:139:GLN:HG2	1:F:175:GLN:NE2	2.30	0.47
1:F:94:VAL:O	1:F:96:GLN:HG2	2.14	0.47
1:A:418:VAL:HG22	1:A:484:ILE:HG21	1.96	0.47
1:G:288:ASN:ND2	1:G:438:ASN:OD1	2.47	0.47
1:G:439:VAL:HG12	1:G:440:PHE:N	2.30	0.47
1:B:410:ALA:HB1	1:B:421:LEU:HD11	1.97	0.47
1:F:200:ALA:HB1	1:F:213:ASN:H	1.80	0.47
1:G:418:VAL:HG11	1:G:484:ILE:HD13	1.96	0.47
1:F:370:ARG:HG3	1:F:386:VAL:HG12	1.96	0.47
1:G:379:ILE:HG21	1:G:386:VAL:CG2	2.17	0.47
1:B:299:GLN:HB2	1:B:302:VAL:HG12	1.96	0.47
1:H:118:SER:O	1:H:121:ALA:HB3	2.15	0.47
1:A:319:TYR:CE1	1:E:390:LEU:HB3	2.50	0.47
1:B:123:LEU:O	1:B:126:VAL:HG22	2.15	0.47
1:B:479:LEU:HD12	1:B:480:PHE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:VAL:HB	1:C:260:VAL:HG21	1.97	0.47
1:F:154:ILE:CG1	1:F:159:ILE:HD11	2.44	0.47
1:F:341:ASP:HB3	1:F:434:ASN:OD1	2.15	0.47
1:B:98:GLN:H	1:B:98:GLN:CD	2.18	0.47
1:D:367:ASP:HA	1:D:370:ARG:NH1	2.30	0.47
1:E:337:GLU:HG2	1:E:343:GLY:HA3	1.97	0.47
1:F:67:THR:N	1:G:67:THR:CG2	2.78	0.47
1:H:90:TYR:CZ	1:H:264:LEU:HD22	2.49	0.47
1:E:287:ILE:HG22	1:E:289:LEU:HD13	1.96	0.47
1:E:457:ASN:HD22	1:E:457:ASN:C	2.19	0.47
1:G:79:SER:OG	1:G:81:LYS:HG3	2.15	0.47
1:A:444:ARG:HG2	1:A:444:ARG:HH11	1.78	0.46
1:C:338:LEU:HD23	1:C:338:LEU:HA	1.67	0.46
1:D:337:GLU:HG2	1:D:343:GLY:HA3	1.97	0.46
1:E:237:LEU:HG	1:E:245:MET:HE2	1.96	0.46
1:F:136:THR:O	1:F:136:THR:CG2	2.59	0.46
1:F:98:GLN:CD	1:F:99:PHE:H	2.18	0.46
1:G:79:SER:C	1:G:81:LYS:N	2.68	0.46
1:D:329:ILE:HG21	1:D:337:GLU:HG3	1.98	0.46
1:F:337:GLU:HG2	1:F:343:GLY:HA3	1.97	0.46
1:G:287:ILE:HG22	1:G:289:LEU:HD13	1.97	0.46
1:G:317:LEU:HA	1:G:320:LEU:HD12	1.96	0.46
1:H:203:LEU:HD12	1:H:203:LEU:O	2.15	0.46
1:D:98:GLN:NE2	1:D:98:GLN:CA	2.64	0.46
1:F:432:LEU:N	1:F:432:LEU:HD23	2.31	0.46
1:C:357:ARG:NH2	1:C:364:PRO:HD3	2.31	0.46
1:A:133:LEU:C	1:A:133:LEU:HD13	2.36	0.46
1:A:316:LEU:HG	1:A:320:LEU:HD11	1.98	0.46
1:B:144:LEU:HD11	1:B:164:THR:HG23	1.97	0.46
1:F:72:ILE:CA	1:G:89:LYS:HZ2	2.28	0.46
1:G:95:SER:CB	1:G:98:GLN:HB2	2.46	0.46
1:A:198:PHE:CD1	1:A:214:ILE:HD13	2.51	0.46
1:B:68:ARG:NH1	1:C:91:PHE:O	2.46	0.46
1:G:74:LEU:CD2	1:G:74:LEU:C	2.84	0.46
1:A:102:ILE:HD12	1:A:130:PRO:HB2	1.98	0.46
1:A:337:GLU:HG2	1:A:343:GLY:HA3	1.97	0.46
1:A:457:ASN:C	1:A:457:ASN:HD22	2.19	0.46
1:B:337:GLU:HG2	1:B:343:GLY:HA3	1.98	0.46
1:C:67:THR:O	1:C:71:VAL:HG23	2.15	0.46
1:D:133:LEU:C	1:D:133:LEU:CD2	2.84	0.46
1:D:249:ASN:HB3	1:D:252:VAL:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:ASN:O	1:H:180:VAL:HG23	2.16	0.46
1:H:454:VAL:HG21	1:H:464:HIS:CG	2.51	0.46
1:A:98:GLN:HE21	1:A:99:PHE:H	1.62	0.46
1:B:424:PHE:HE1	1:B:439:VAL:HG11	1.81	0.46
1:B:437:ASP:O	1:B:441:ASN:ND2	2.49	0.46
1:C:486:ASP:OD2	1:C:489:THR:HG23	2.16	0.46
1:C:492:GLU:O	1:C:496:ASN:ND2	2.48	0.46
1:E:275:ILE:CG2	1:E:284:ILE:HD12	2.44	0.46
1:G:79:SER:O	1:G:81:LYS:N	2.49	0.46
1:G:79:SER:CB	1:G:84:VAL:HG21	2.44	0.46
1:H:87:TYR:CD2	1:H:339:PHE:O	2.69	0.46
1:B:146:ALA:O	1:E:474:LYS:NZ	2.47	0.46
1:D:473:LEU:HD13	1:D:478:VAL:HG22	1.98	0.46
1:F:418:VAL:HG11	1:F:451:GLN:HB3	1.98	0.46
1:G:160:THR:HG21	1:G:165:MET:CE	2.35	0.46
1:A:259:ARG:HD3	1:E:391:ARG:HE	1.81	0.46
1:A:259:ARG:O	1:E:387:ALA:HB3	2.16	0.46
1:C:94:VAL:CG1	1:C:98:GLN:OE1	2.60	0.46
1:G:131:ILE:HD13	1:G:222:ILE:HG21	1.97	0.46
1:B:146:ALA:O	1:E:474:LYS:CE	2.64	0.45
1:D:412:VAL:HG11	1:D:447:PHE:CE1	2.51	0.45
1:A:317:LEU:HD23	1:A:320:LEU:HD12	1.98	0.45
1:A:369:LEU:HD22	1:A:373:LEU:HD11	1.98	0.45
1:C:474:LYS:HD3	1:C:498:VAL:HG22	1.97	0.45
1:F:94:VAL:O	1:F:95:SER:C	2.53	0.45
1:G:299:GLN:O	1:G:302:VAL:HG12	2.17	0.45
1:B:276:ILE:CD1	1:B:283:LYS:HG3	2.46	0.45
1:C:267:VAL:HG21	1:C:338:LEU:HD21	1.98	0.45
1:C:286:MET:CE	1:C:288:ASN:OD1	2.65	0.45
1:G:337:GLU:HG2	1:G:343:GLY:HA3	1.97	0.45
1:H:136:THR:HG23	1:H:136:THR:O	2.17	0.45
1:D:442:VAL:HG13	1:D:445:ARG:HH12	1.79	0.45
1:E:242:SER:HB3	1:F:162:GLU:HG2	1.97	0.45
1:C:369:LEU:CD2	1:C:373:LEU:HD11	2.41	0.45
1:E:245:MET:HG3	1:F:243:GLY:O	2.16	0.45
1:F:354:LEU:HD12	1:F:442:VAL:HG21	1.97	0.45
1:E:431:TRP:CE2	1:E:436:THR:HG21	2.52	0.45
1:G:211:VAL:CG1	1:G:212:GLY:N	2.79	0.45
1:H:106:GLY:C	1:H:139:GLN:HE22	2.20	0.45
1:A:434:ASN:N	1:A:434:ASN:OD1	2.49	0.45
1:G:84:VAL:HG13	1:G:339:PHE:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:MET:HE2	1:H:310:ILE:HG22	1.98	0.45
1:D:370:ARG:CG	1:D:386:VAL:HG11	2.35	0.45
1:D:147:GLN:CG	1:G:321:PRO:HG3	2.46	0.45
1:B:169:ARG:NH1	1:B:245:MET:CE	2.80	0.45
1:C:112:ASN:HD22	1:C:115:GLU:HB2	1.82	0.45
1:C:291:GLU:OE2	1:C:442:VAL:CG2	2.60	0.45
1:C:86:GLN:O	1:C:90:TYR:HD2	2.00	0.45
1:E:401:TYR:CD2	1:E:442:VAL:HG11	2.52	0.45
1:F:322:ARG:NH1	1:F:350:ARG:CZ	2.80	0.45
1:F:404:GLU:N	1:F:405:PRO:CD	2.80	0.45
1:G:217:VAL:HB	1:G:260:VAL:HG21	1.99	0.45
1:H:113:LEU:HD21	1:H:182:ALA:CB	2.47	0.45
1:H:407:GLU:OE2	1:H:429:ALA:HB3	2.17	0.45
1:A:242:SER:HB3	1:B:162:GLU:HG3	1.97	0.44
1:C:337:GLU:HG2	1:C:343:GLY:HA3	1.99	0.44
1:B:491:SER:HA	1:C:487:ILE:HD11	1.99	0.44
1:C:78:ILE:HA	1:C:83:GLU:OE1	2.16	0.44
1:D:469:GLN:HE21	1:D:469:GLN:HB2	1.56	0.44
1:F:313:ILE:HD13	1:F:348:ILE:HD13	2.00	0.44
1:G:233:ILE:HD12	1:G:233:ILE:HG23	1.60	0.44
1:B:144:LEU:HA	1:B:144:LEU:HD23	1.76	0.44
1:B:313:ILE:HD13	1:B:348:ILE:HD13	2.00	0.44
1:C:99:PHE:HZ	1:C:338:LEU:HD13	1.81	0.44
1:B:71:VAL:HG13	1:C:74:LEU:CD2	2.47	0.44
1:A:404:GLU:OE2	1:E:367:ASP:HB3	2.17	0.44
1:G:258:ALA:HB1	1:G:266:ILE:HD13	1.99	0.44
1:G:486:ASP:OD2	1:G:489:THR:HG23	2.18	0.44
1:B:74:LEU:CD1	1:B:78:ILE:HD11	2.45	0.44
1:C:249:ASN:HB3	1:C:252:VAL:CG2	2.47	0.44
1:H:354:LEU:HA	1:H:354:LEU:HD23	1.68	0.44
1:D:474:LYS:HD3	1:D:498:VAL:HG13	1.98	0.44
1:A:391:ARG:HA	1:E:319:TYR:CE2	2.53	0.44
1:G:404:GLU:N	1:G:405:PRO:CD	2.80	0.44
1:B:412:VAL:HG11	1:B:447:PHE:CZ	2.52	0.44
1:F:341:ASP:HB2	1:F:434:ASN:CG	2.37	0.44
1:F:80:THR:CG2	1:F:81:LYS:N	2.81	0.44
1:C:176:ASN:HD21	1:C:192:PRO:CB	2.30	0.44
1:C:275:ILE:HD12	1:C:346:THR:HG21	1.99	0.44
1:G:332:GLN:O	1:G:335:GLN:NE2	2.40	0.44
1:H:116:LEU:HD22	1:H:120:LEU:CD1	2.47	0.44
1:H:428:ASP:OD1	1:H:428:ASP:N	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLN:HG2	1:D:175:GLN:CD	2.37	0.44
1:E:260:VAL:HG12	1:E:261:PHE:N	2.33	0.44
1:E:431:TRP:CE3	1:E:460:ASN:ND2	2.85	0.44
1:G:80:THR:O	1:G:80:THR:HG23	2.13	0.44
1:H:275:ILE:CG2	1:H:284:ILE:HD12	2.46	0.44
1:B:144:LEU:HD21	1:B:167:VAL:HG21	1.99	0.44
1:B:269:LEU:HD22	1:B:331:VAL:HA	2.00	0.44
1:D:119:CYS:SG	1:D:334:LEU:HD13	2.57	0.44
1:E:456:GLU:OE2	1:E:473:LEU:HD21	2.18	0.44
1:E:360:ILE:HD11	1:E:393:LEU:CD1	2.48	0.44
1:G:97:GLN:HB2	1:G:226:ILE:HG21	2.00	0.44
1:G:329:ILE:HG22	1:G:345:GLY:HA3	1.99	0.44
1:H:335:GLN:N	1:H:335:GLN:HE21	2.14	0.44
1:A:260:VAL:CG1	1:A:261:PHE:CD2	2.96	0.43
1:B:214:ILE:HD11	1:B:248:VAL:HG11	1.99	0.43
1:B:379:ILE:HG21	1:B:386:VAL:HG22	1.84	0.43
1:C:331:VAL:O	1:C:334:LEU:HB2	2.18	0.43
1:C:431:TRP:CD2	1:C:436:THR:HG21	2.52	0.43
1:C:488:ASN:C	1:C:488:ASN:HD22	2.21	0.43
1:D:432:LEU:N	1:D:432:LEU:HD23	2.33	0.43
1:E:347:MET:HB2	1:E:347:MET:HE3	1.66	0.43
1:F:320:LEU:HB3	1:F:321:PRO:HD2	1.98	0.43
1:A:260:VAL:HG12	1:A:261:PHE:CG	2.52	0.43
1:F:72:ILE:HA	1:G:89:LYS:HZ2	1.83	0.43
1:G:94:VAL:O	1:G:94:VAL:CG1	2.65	0.43
1:A:275:ILE:HG22	1:A:284:ILE:HD12	2.00	0.43
1:C:437:ASP:O	1:C:441:ASN:ND2	2.51	0.43
1:D:171:CYS:O	1:D:175:GLN:HG2	2.18	0.43
1:F:392:TYR:CD1	1:F:392:TYR:O	2.72	0.43
1:F:74:LEU:CD1	1:G:71:VAL:HG13	2.48	0.43
1:G:154:ILE:CG1	1:G:159:ILE:HD11	2.43	0.43
1:H:121:ALA:HA	1:H:188:VAL:HG21	1.99	0.43
1:H:140:VAL:HG22	1:H:171:CYS:CB	2.48	0.43
1:F:428:ASP:N	1:F:428:ASP:OD1	2.42	0.43
1:G:90:TYR:OH	1:G:323:SER:CB	2.65	0.43
1:G:349:ARG:HH11	1:G:349:ARG:HB2	1.82	0.43
1:G:93:SER:O	1:G:94:VAL:CG2	2.66	0.43
1:C:404:GLU:N	1:C:405:PRO:CD	2.81	0.43
1:G:130:PRO:HD2	1:G:231:LEU:HD21	2.01	0.43
1:G:418:VAL:HG21	1:G:484:ILE:HD13	2.00	0.43
1:A:124:TYR:CD2	1:A:188:VAL:HG13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:ASN:HD21	1:F:251:ASP:HB2	1.84	0.43
1:G:426:CYS:SG	1:G:431:TRP:NE1	2.91	0.43
1:H:317:LEU:HD13	1:H:349:ARG:HA	2.01	0.43
1:H:88:LEU:HD23	1:H:88:LEU:HA	1.74	0.43
1:B:169:ARG:HH11	1:B:245:MET:CE	2.31	0.43
1:B:401:TYR:CE2	1:B:442:VAL:CG1	3.02	0.43
1:B:494:VAL:O	1:B:498:VAL:HG23	2.18	0.43
1:C:355:VAL:HB	1:C:357:ARG:HH11	1.82	0.43
1:D:454:VAL:HG21	1:D:464:HIS:CG	2.53	0.43
1:D:486:ASP:OD2	1:D:489:THR:HG23	2.18	0.43
1:H:116:LEU:HD22	1:H:120:LEU:HD12	2.00	0.43
1:H:144:LEU:HD23	1:H:167:VAL:HG21	2.01	0.43
1:H:357:ARG:HH12	1:H:402:ALA:HB3	1.84	0.43
1:B:232:PRO:O	1:B:233:ILE:HD13	2.19	0.43
1:C:367:ASP:HA	1:C:370:ARG:HH12	1.83	0.43
1:C:94:VAL:CG2	1:C:98:GLN:OE1	2.65	0.43
1:D:157:ILE:HD13	1:D:208:TYR:CZ	2.53	0.43
1:H:113:LEU:CD2	1:H:182:ALA:CB	2.96	0.43
1:A:334:LEU:HD23	1:A:334:LEU:O	2.19	0.43
1:B:144:LEU:HD22	1:B:149:ILE:HD12	2.01	0.43
1:C:449:ALA:CB	1:C:484:ILE:HG23	2.48	0.43
1:D:430:ALA:HA	1:D:435:VAL:HG11	2.01	0.43
1:E:449:ALA:CB	1:E:484:ILE:HG23	2.46	0.43
1:F:317:LEU:HD13	1:F:349:ARG:HA	2.00	0.43
1:A:232:PRO:O	1:A:233:ILE:HD13	2.19	0.42
1:A:239:GLU:HG3	1:B:169:ARG:NH2	2.30	0.42
1:A:287:ILE:HG22	1:A:289:LEU:HD13	2.01	0.42
1:G:121:ALA:HA	1:G:188:VAL:HG21	2.00	0.42
1:A:329:ILE:HD12	1:A:334:LEU:HA	2.01	0.42
1:B:123:LEU:HD11	1:B:338:LEU:CD1	2.48	0.42
1:D:147:GLN:HA	1:G:321:PRO:CB	2.50	0.42
1:D:286:MET:HE2	1:D:438:ASN:ND2	2.28	0.42
1:E:338:LEU:HD23	1:E:338:LEU:HA	1.92	0.42
1:F:370:ARG:HG3	1:F:386:VAL:CG1	2.50	0.42
1:G:97:GLN:C	1:G:99:PHE:N	2.72	0.42
1:A:334:LEU:C	1:A:334:LEU:CD2	2.88	0.42
1:E:101:VAL:HG23	1:E:263:PRO:HG3	2.01	0.42
1:A:370:ARG:CZ	1:E:321:PRO:HG3	2.48	0.42
1:E:434:ASN:OD1	1:E:434:ASN:N	2.52	0.42
1:E:493:LEU:HD12	1:E:493:LEU:HA	1.65	0.42
1:F:70:THR:HG23	1:F:122:PHE:HD1	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:ARG:HD3	1:F:460:ASN:HD22	1.84	0.42
1:G:264:LEU:HD22	1:G:323:SER:OG	2.19	0.42
1:G:95:SER:HB3	1:G:98:GLN:CB	2.48	0.42
1:H:456:GLU:OE2	1:H:473:LEU:HD21	2.19	0.42
1:B:404:GLU:N	1:B:405:PRO:CD	2.82	0.42
1:C:276:ILE:HD11	1:C:283:LYS:HD3	2.01	0.42
1:C:286:MET:HE3	1:C:288:ASN:OD1	2.20	0.42
1:B:84:VAL:HG13	1:C:75:LEU:HD22	2.01	0.42
1:D:404:GLU:N	1:D:405:PRO:CD	2.82	0.42
1:D:494:VAL:O	1:D:498:VAL:HG23	2.19	0.42
1:F:354:LEU:HD23	1:F:354:LEU:HA	1.76	0.42
1:G:91:PHE:HE1	1:G:264:LEU:HB3	1.83	0.42
1:H:160:THR:HG21	1:H:165:MET:CE	2.49	0.42
1:H:337:GLU:HG2	1:H:343:GLY:HA3	2.00	0.42
1:B:136:THR:HG22	1:B:172:PHE:CZ	2.54	0.42
1:C:484:ILE:HD13	1:C:484:ILE:HG21	1.81	0.42
1:D:231:LEU:HA	1:D:231:LEU:HD23	1.63	0.42
1:D:286:MET:HG3	1:D:437:ASP:CB	2.50	0.42
1:D:473:LEU:HD12	1:D:477:LYS:O	2.19	0.42
1:E:404:GLU:N	1:E:405:PRO:CD	2.83	0.42
1:F:76:ASN:HB2	1:F:77:ASN:ND2	2.34	0.42
1:B:169:ARG:NH1	1:B:245:MET:HE3	2.34	0.42
1:C:103:LYS:NZ	1:C:251:ASP:OD1	2.44	0.42
1:D:286:MET:HE2	1:D:438:ASN:HD22	1.83	0.42
1:E:113:LEU:HA	1:E:113:LEU:HD12	1.77	0.42
1:F:203:LEU:HD23	1:F:208:TYR:CD2	2.55	0.42
1:G:264:LEU:N	1:G:264:LEU:HD23	2.34	0.42
1:C:487:ILE:O	1:C:487:ILE:HD12	2.20	0.42
1:D:303:LYS:HD2	1:D:304:TYR:H	1.83	0.42
1:E:421:LEU:HA	1:E:421:LEU:HD12	1.70	0.42
1:G:454:VAL:HG21	1:G:464:HIS:CD2	2.55	0.42
1:G:454:VAL:HG21	1:G:464:HIS:CG	2.55	0.42
1:A:454:VAL:HG12	1:A:455:SER:N	2.34	0.42
1:E:316:LEU:HG	1:E:320:LEU:HD11	2.01	0.42
1:E:354:LEU:CD1	1:E:439:VAL:HG22	2.49	0.42
1:E:370:ARG:O	1:E:374:GLN:HG2	2.19	0.42
1:G:403:ASP:N	1:G:403:ASP:OD1	2.51	0.42
1:H:473:LEU:HD12	1:H:477:LYS:O	2.20	0.42
1:A:404:GLU:N	1:A:405:PRO:CD	2.83	0.42
1:D:367:ASP:HA	1:D:370:ARG:HH12	1.85	0.42
1:D:430:ALA:CB	1:D:435:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:303:LYS:HD2	1:F:304:TYR:H	1.85	0.42
1:H:231:LEU:HD23	1:H:231:LEU:HA	1.76	0.42
1:H:419:PRO:O	1:H:450:LEU:HD12	2.20	0.42
1:H:133:LEU:C	1:H:133:LEU:HD23	2.41	0.42
1:A:379:ILE:HG21	1:A:386:VAL:HG23	2.02	0.41
1:B:133:LEU:HD11	1:B:236:SER:HB3	2.02	0.41
1:F:442:VAL:HG13	1:F:445:ARG:HH11	1.84	0.41
1:H:457:ASN:ND2	1:H:457:ASN:O	2.46	0.41
1:C:218:THR:HG22	1:C:220:GLU:HG2	2.01	0.41
1:C:232:PRO:C	1:C:233:ILE:HD13	2.39	0.41
1:C:93:SER:CB	1:C:95:SER:H	2.33	0.41
1:E:193:ILE:HB	1:E:234:LEU:HD13	2.02	0.41
1:F:94:VAL:CG1	1:F:94:VAL:O	2.67	0.41
1:G:79:SER:HG	1:G:84:VAL:HG21	1.78	0.41
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.68	0.41
1:B:259:ARG:CG	1:B:319:TYR:CE1	3.03	0.41
1:C:432:LEU:N	1:C:432:LEU:HD23	2.35	0.41
1:G:372:ALA:O	1:G:375:ARG:HD2	2.20	0.41
1:B:73:GLN:NE2	1:B:335:GLN:HG2	2.34	0.41
1:C:270:ASN:ND2	1:C:272:LYS:HD3	2.35	0.41
1:C:284:ILE:HD11	1:C:301:TRP:CH2	2.55	0.41
1:G:136:THR:CG2	1:G:136:THR:O	2.60	0.41
1:H:232:PRO:O	1:H:233:ILE:HD13	2.20	0.41
1:B:104:VAL:HG12	1:B:105:GLY:O	2.20	0.41
1:B:296:LEU:HD12	1:B:296:LEU:HA	1.69	0.41
1:B:370:ARG:O	1:B:374:GLN:HG2	2.20	0.41
1:C:87:TYR:CZ	1:C:339:PHE:HB2	2.55	0.41
1:G:430:ALA:HA	1:G:435:VAL:CG1	2.51	0.41
1:F:494:VAL:CG1	1:G:487:ILE:HD12	2.50	0.41
1:H:461:ILE:CG2	1:H:462:ALA:N	2.84	0.41
1:B:421:LEU:HB3	1:B:452:TRP:HB3	2.02	0.41
1:C:501:CYS:O	1:C:502:ASP:CB	2.65	0.41
1:F:104:VAL:HG12	1:F:105:GLY:O	2.20	0.41
1:B:434:ASN:N	1:B:434:ASN:OD1	2.53	0.41
1:C:456:GLU:OE2	1:C:473:LEU:HD21	2.20	0.41
1:D:259:ARG:HD3	1:D:319:TYR:CE2	2.55	0.41
1:F:454:VAL:HG12	1:F:455:SER:N	2.36	0.41
1:F:67:THR:N	1:G:67:THR:HG22	2.35	0.41
1:A:320:LEU:HB3	1:A:321:PRO:HD2	2.02	0.41
1:A:332:GLN:HG3	1:A:333:ASP:OD1	2.21	0.41
1:B:331:VAL:HG13	1:B:332:GLN:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HD23	1:C:128:LEU:HA	1.66	0.41
1:D:248:VAL:N	2:D:1503:NLG:H8C2	2.36	0.41
1:G:338:LEU:HD23	1:G:338:LEU:HA	1.70	0.41
1:D:412:VAL:HG11	1:D:447:PHE:CZ	2.56	0.41
1:E:442:VAL:HG12	1:E:443:LEU:N	2.33	0.41
1:E:455:SER:O	1:E:461:ILE:HD13	2.21	0.41
1:H:124:TYR:CG	1:H:188:VAL:HG13	2.56	0.41
1:H:402:ALA:HB1	1:H:406:LEU:HD23	2.01	0.41
1:A:283:LYS:HZ1	1:A:345:GLY:N	2.19	0.41
1:E:451:GLN:NE2	1:E:493:LEU:HD11	2.36	0.41
1:F:455:SER:O	1:F:461:ILE:HD13	2.20	0.41
1:G:412:VAL:HG11	1:G:447:PHE:CE1	2.55	0.41
1:C:379:ILE:HD11	1:C:423:LYS:HZ1	1.84	0.41
1:C:393:LEU:HD23	1:C:393:LEU:HA	1.88	0.41
1:D:434:ASN:OD1	1:D:434:ASN:N	2.54	0.41
1:H:484:ILE:HD11	1:H:493:LEU:CD2	2.50	0.41
1:B:368:ALA:CB	1:B:406:LEU:HD13	2.48	0.40
1:F:133:LEU:HD12	1:F:257:LEU:HD12	2.02	0.40
1:H:140:VAL:HG22	1:H:171:CYS:HB2	2.02	0.40
1:H:320:LEU:HB3	1:H:321:PRO:HD2	2.02	0.40
1:A:180:VAL:HG13	1:A:190:ALA:CB	2.48	0.40
1:A:317:LEU:HD23	1:A:320:LEU:CD1	2.51	0.40
1:A:494:VAL:O	1:A:498:VAL:HG23	2.22	0.40
1:B:144:LEU:HD23	1:B:167:VAL:HG21	2.03	0.40
1:B:329:ILE:CG2	1:B:337:GLU:HG3	2.51	0.40
1:C:370:ARG:O	1:C:374:GLN:HG2	2.21	0.40
1:C:461:ILE:O	1:C:461:ILE:HD13	2.21	0.40
1:F:403:ASP:N	1:F:403:ASP:OD1	2.55	0.40
1:F:435:VAL:O	1:F:435:VAL:HG23	2.18	0.40
1:A:179:LEU:O	1:A:183:LEU:HD12	2.22	0.40
1:B:329:ILE:HG21	1:B:337:GLU:HG3	2.02	0.40
1:C:220:GLU:N	1:C:221:PRO:CD	2.85	0.40
1:E:320:LEU:HB3	1:E:321:PRO:HD2	2.04	0.40
1:F:488:ASN:C	1:F:488:ASN:HD22	2.25	0.40
1:A:139:GLN:HE21	1:A:175:GLN:CD	2.24	0.40
1:A:201:ASP:N	1:A:201:ASP:OD1	2.54	0.40
1:B:490:ILE:O	1:B:494:VAL:HG23	2.21	0.40
1:C:119:CYS:SG	1:C:334:LEU:HB3	2.62	0.40
1:D:203:LEU:HD23	1:D:208:TYR:CE2	2.56	0.40
1:D:351:GLY:C	1:D:352:TYR:CD1	2.94	0.40
1:D:418:VAL:HG21	1:D:484:ILE:CD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:ASP:HA	1:F:347:MET:HE1	2.03	0.40
1:G:257:LEU:HA	1:G:257:LEU:HD23	1.85	0.40
1:H:155:ASP:HA	1:H:304:TYR:CE2	2.57	0.40
1:A:334:LEU:C	1:A:334:LEU:HD23	2.41	0.40
1:A:393:LEU:HD11	1:A:411:ILE:HD13	2.02	0.40
1:C:136:THR:HG23	1:C:136:THR:O	2.22	0.40
1:C:164:THR:O	1:C:168:VAL:HG23	2.22	0.40
1:C:237:LEU:HD12	1:C:237:LEU:HA	1.87	0.40

All (3) 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:A:488:ASN:OD1	1:H:362:GLU:OE2[1_554]	1.75	0.45
1:E:207:LYS:NZ	1:G:282:GLU:OE2[1_545]	2.14	0.06
1:C:146:ALA:O	1:F:433:ASN:ND2[1_655]	2.19	0.01

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	403/464 (87%)	371 (92%)	29 (7%)	3 (1%)	25	65
1	B	434/464 (94%)	397 (92%)	32 (7%)	5 (1%)	15	54
1	C	434/464 (94%)	397 (92%)	33 (8%)	4 (1%)	20	60
1	D	403/464 (87%)	370 (92%)	31 (8%)	2 (0%)	32	71
1	E	403/464 (87%)	369 (92%)	31 (8%)	3 (1%)	25	65
1	F	434/464 (94%)	395 (91%)	36 (8%)	3 (1%)	25	65
1	G	434/464 (94%)	392 (90%)	36 (8%)	6 (1%)	13	50
1	H	420/464 (90%)	386 (92%)	30 (7%)	4 (1%)	18	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3365/3712 (91%)	3077 (91%)	258 (8%)	30 (1%)	20 60

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	THR
1	A	487	ILE
1	B	416	THR
1	C	93	SER
1	C	416	THR
1	D	416	THR
1	E	416	THR
1	F	416	THR
1	G	94	VAL
1	G	98	GLN
1	G	416	THR
1	H	416	THR
1	A	434	ASN
1	B	93	SER
1	B	434	ASN
1	B	487	ILE
1	C	434	ASN
1	C	487	ILE
1	D	487	ILE
1	E	434	ASN
1	F	434	ASN
1	F	487	ILE
1	G	97	GLN
1	H	434	ASN
1	H	487	ILE
1	B	321	PRO
1	E	487	ILE
1	G	487	ILE
1	H	344	ALA
1	G	95	SER

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	340/397 (86%)	300 (88%)	40 (12%)	6	27
1	B	371/397 (94%)	328 (88%)	43 (12%)	6	27
1	C	370/397 (93%)	333 (90%)	37 (10%)	9	34
1	D	340/397 (86%)	299 (88%)	41 (12%)	6	25
1	E	340/397 (86%)	307 (90%)	33 (10%)	9	35
1	F	372/397 (94%)	334 (90%)	38 (10%)	8	33
1	G	370/397 (93%)	331 (90%)	39 (10%)	8	32
1	H	355/397 (89%)	312 (88%)	43 (12%)	6	25
All	All	2858/3176 (90%)	2544 (89%)	314 (11%)	7	30

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	177	LEU
1	A	199	THR
1	A	201	ASP
1	A	206	ASP
1	A	209	LYS
1	A	215	LYS
1	A	220	GLU
1	A	239	GLU
1	A	260	VAL
1	A	271	GLU
1	A	283	LYS
1	A	289	LEU
1	A	295	ASP
1	A	298	LYS
1	A	308	LEU
1	A	329	ILE
1	A	333	ASP
1	A	334	LEU
1	A	335	GLN
1	A	341	ASP
1	A	349	ARG
1	A	370	ARG
1	A	383	LYS

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Mol	Chain	Res	Type
1	A	386	VAL
1	A	393	LEU
1	A	396	SER
1	A	423	LYS
1	A	428	ASP
1	A	434	ASN
1	A	435	VAL
1	A	440	PHE
1	A	443	LEU
1	A	444	ARG
1	A	457	ASN
1	A	460	ASN
1	A	469	GLN
1	A	488	ASN
1	A	491	SER
1	A	499	LYS
1	B	67	THR
1	B	69	SER
1	B	79	SER
1	B	80	THR
1	B	82	ARG
1	B	169	ARG
1	B	175	GLN
1	B	199	THR
1	B	203	LEU
1	B	206	ASP
1	B	209	LYS
1	B	215	LYS
1	B	220	GLU
1	B	256	GLU
1	B	271	GLU
1	B	283	LYS
1	B	286	MET
1	B	289	LEU
1	B	295	ASP
1	B	316	LEU
1	B	329	ILE
1	B	333	ASP
1	B	334	LEU
1	B	335	GLN
1	B	341	ASP
1	B	349	ARG

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Mol	Chain	Res	Type
1	B	369	LEU
1	B	370	ARG
1	B	383	LYS
1	B	396	SER
1	B	404	GLU
1	B	428	ASP
1	B	434	ASN
1	B	440	PHE
1	B	443	LEU
1	B	444	ARG
1	B	457	ASN
1	B	460	ASN
1	B	469	GLN
1	B	474	LYS
1	B	488	ASN
1	B	491	SER
1	B	499	LYS
1	C	67	THR
1	C	69	SER
1	C	79	SER
1	C	80	THR
1	C	93	SER
1	C	95	SER
1	C	115	GLU
1	C	118	SER
1	C	175	GLN
1	C	177	LEU
1	C	199	THR
1	C	206	ASP
1	C	220	GLU
1	C	239	GLU
1	C	271	GLU
1	C	272	LYS
1	C	289	LEU
1	C	295	ASP
1	C	329	ILE
1	C	333	ASP
1	C	335	GLN
1	C	341	ASP
1	C	393	LEU
1	C	396	SER
1	C	428	ASP

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Mol	Chain	Res	Type
1	C	434	ASN
1	C	440	PHE
1	C	443	LEU
1	C	444	ARG
1	C	457	ASN
1	C	458	ASP
1	C	460	ASN
1	C	461	ILE
1	C	469	GLN
1	C	488	ASN
1	C	491	SER
1	C	499	LYS
1	D	98	GLN
1	D	113	LEU
1	D	115	GLU
1	D	133	LEU
1	D	143	ARG
1	D	168	VAL
1	D	199	THR
1	D	206	ASP
1	D	215	LYS
1	D	220	GLU
1	D	239	GLU
1	D	271	GLU
1	D	283	LYS
1	D	288	ASN
1	D	295	ASP
1	D	303	LYS
1	D	304	TYR
1	D	312	GLU
1	D	329	ILE
1	D	333	ASP
1	D	334	LEU
1	D	341	ASP
1	D	349	ARG
1	D	352	TYR
1	D	367	ASP
1	D	369	LEU
1	D	396	SER
1	D	404	GLU
1	D	428	ASP
1	D	434	ASN

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Mol	Chain	Res	Type
1	D	440	PHE
1	D	443	LEU
1	D	444	ARG
1	D	457	ASN
1	D	460	ASN
1	D	469	GLN
1	D	478	VAL
1	D	488	ASN
1	D	491	SER
1	D	493	LEU
1	D	499	LYS
1	E	143	ARG
1	E	175	GLN
1	E	199	THR
1	E	206	ASP
1	E	209	LYS
1	E	215	LYS
1	E	220	GLU
1	E	239	GLU
1	E	248	VAL
1	E	271	GLU
1	E	289	LEU
1	E	295	ASP
1	E	320	LEU
1	E	329	ILE
1	E	333	ASP
1	E	334	LEU
1	E	335	GLN
1	E	341	ASP
1	E	349	ARG
1	E	375	ARG
1	E	383	LYS
1	E	396	SER
1	E	428	ASP
1	E	435	VAL
1	E	440	PHE
1	E	443	LEU
1	E	444	ARG
1	E	457	ASN
1	E	460	ASN
1	E	469	GLN
1	E	488	ASN

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Mol	Chain	Res	Type
1	E	491	SER
1	E	499	LYS
1	F	67	THR
1	F	69	SER
1	F	73	GLN
1	F	79	SER
1	F	113	LEU
1	F	114	HIS
1	F	115	GLU
1	F	133	LEU
1	F	173	LEU
1	F	175	GLN
1	F	199	THR
1	F	206	ASP
1	F	209	LYS
1	F	215	LYS
1	F	220	GLU
1	F	271	GLU
1	F	283	LYS
1	F	295	ASP
1	F	329	ILE
1	F	333	ASP
1	F	334	LEU
1	F	341	ASP
1	F	369	LEU
1	F	383	LYS
1	F	396	SER
1	F	404	GLU
1	F	428	ASP
1	F	434	ASN
1	F	440	PHE
1	F	443	LEU
1	F	444	ARG
1	F	457	ASN
1	F	458	ASP
1	F	460	ASN
1	F	469	GLN
1	F	488	ASN
1	F	491	SER
1	F	499	LYS
1	G	67	THR
1	G	69	SER

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Mol	Chain	Res	Type
1	G	79	SER
1	G	80	THR
1	G	88	LEU
1	G	97	GLN
1	G	115	GLU
1	G	175	GLN
1	G	199	THR
1	G	206	ASP
1	G	215	LYS
1	G	220	GLU
1	G	239	GLU
1	G	271	GLU
1	G	283	LYS
1	G	286	MET
1	G	289	LEU
1	G	308	LEU
1	G	320	LEU
1	G	329	ILE
1	G	333	ASP
1	G	335	GLN
1	G	341	ASP
1	G	349	ARG
1	G	370	ARG
1	G	393	LEU
1	G	396	SER
1	G	407	GLU
1	G	428	ASP
1	G	434	ASN
1	G	439	VAL
1	G	440	PHE
1	G	443	LEU
1	G	444	ARG
1	G	457	ASN
1	G	469	GLN
1	G	488	ASN
1	G	491	SER
1	G	499	LYS
1	H	92	THR
1	H	93	SER
1	H	94	VAL
1	H	97	GLN
1	H	113	LEU

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Mol	Chain	Res	Type
1	H	114	HIS
1	H	115	GLU
1	H	116	LEU
1	H	133	LEU
1	H	175	GLN
1	H	199	THR
1	H	206	ASP
1	H	215	LYS
1	H	220	GLU
1	H	271	GLU
1	H	283	LYS
1	H	291	GLU
1	H	295	ASP
1	H	296	LEU
1	H	303	LYS
1	H	308	LEU
1	H	312	GLU
1	H	333	ASP
1	H	334	LEU
1	H	335	GLN
1	H	341	ASP
1	H	347	MET
1	H	370	ARG
1	H	383	LYS
1	H	396	SER
1	H	404	GLU
1	H	428	ASP
1	H	432	LEU
1	H	434	ASN
1	H	440	PHE
1	H	443	LEU
1	H	444	ARG
1	H	457	ASN
1	H	460	ASN
1	H	469	GLN
1	H	488	ASN
1	H	491	SER
1	H	499	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	GLN
1	A	112	ASN
1	A	175	GLN
1	A	176	ASN
1	A	374	GLN
1	A	438	ASN
1	A	469	GLN
1	A	488	ASN
1	A	496	ASN
1	B	98	GLN
1	B	176	ASN
1	B	249	ASN
1	B	441	ASN
1	B	457	ASN
1	B	488	ASN
1	C	73	GLN
1	C	112	ASN
1	C	147	GLN
1	C	175	GLN
1	C	176	ASN
1	C	374	GLN
1	C	441	ASN
1	C	457	ASN
1	C	488	ASN
1	C	496	ASN
1	D	98	GLN
1	D	112	ASN
1	D	147	GLN
1	D	163	HIS
1	D	176	ASN
1	D	288	ASN
1	D	335	GLN
1	D	374	GLN
1	D	433	ASN
1	D	438	ASN
1	D	457	ASN
1	D	488	ASN
1	E	112	ASN
1	E	176	ASN
1	E	374	GLN
1	E	438	ASN
1	E	451	GLN
1	E	457	ASN

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Mol	Chain	Res	Type
1	E	488	ASN
1	F	77	ASN
1	F	98	GLN
1	F	112	ASN
1	F	125	HIS
1	F	175	GLN
1	F	176	ASN
1	F	249	ASN
1	F	335	GLN
1	F	374	GLN
1	F	433	ASN
1	F	434	ASN
1	F	457	ASN
1	F	460	ASN
1	F	488	ASN
1	G	76	ASN
1	G	176	ASN
1	G	374	GLN
1	G	488	ASN
1	G	496	ASN
1	H	86	GLN
1	H	97	GLN
1	H	112	ASN
1	H	176	ASN
1	H	335	GLN
1	H	374	GLN
1	H	438	ASN
1	H	441	ASN
1	H	488	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 (i)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	NLG	D	1503	-	6,12,12	2.69	3 (50%)	6,15,15	3.79	5 (83%)
2	NLG	H	1503	-	6,12,12	1.96	1 (16%)	6,15,15	1.73	1 (16%)

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
2	NLG	D	1503	-	-	0/7/13/13	0/0/0/0
2	NLG	H	1503	-	-	0/7/13/13	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1503	NLG	C8-C7	-5.67	1.38	1.50
2	H	1503	NLG	C8-C7	-4.53	1.40	1.50
2	D	1503	NLG	CA-N2	2.18	1.49	1.46
2	D	1503	NLG	CB-CA	2.37	1.56	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1503	NLG	CB-CA-C	-4.83	105.27	112.28
2	H	1503	NLG	O7-C7-C8	-2.93	116.72	122.06
2	D	1503	NLG	O7-C7-C8	-2.39	117.71	122.06
2	D	1503	NLG	CG-CB-CA	-2.02	109.14	113.19
2	D	1503	NLG	C8-C7-N2	2.92	121.39	116.11
2	D	1503	NLG	CB-CA-N2	6.64	120.31	110.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1503	NLG	10	0
2	H	1503	NLG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	405/464 (87%)	-0.33	1 (0%)	94	94	46, 81, 135, 187	0
1	B	436/464 (93%)	-0.27	7 (1%)	72	63	37, 73, 149, 245	0
1	C	436/464 (93%)	-0.31	7 (1%)	72	63	35, 73, 151, 219	0
1	D	405/464 (87%)	-0.27	3 (0%)	87	83	45, 80, 142, 205	0
1	E	405/464 (87%)	0.10	17 (4%)	37	29	55, 103, 230, 344	0
1	F	436/464 (93%)	-0.27	5 (1%)	80	73	45, 83, 151, 217	0
1	G	436/464 (93%)	-0.01	22 (5%)	30	21	53, 96, 184, 263	0
1	H	422/464 (90%)	-0.12	9 (2%)	64	54	50, 86, 170, 237	0
All	All	3381/3712 (91%)	-0.19	71 (2%)	64	54	35, 84, 166, 344	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	96	GLN	7.8
1	G	383	LYS	7.8
1	B	380	SER	6.7
1	G	381	SER	6.5
1	E	341	ASP	6.3
1	B	379	ILE	6.0
1	E	305	GLY	5.9
1	H	381	SER	5.7
1	G	279	SER	5.7
1	C	383	LYS	5.6
1	H	377	ALA	4.9
1	G	300	SER	4.9
1	H	383	LYS	4.8
1	E	342	SER	4.5
1	E	381	SER	4.4
1	F	381	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	381	SER	4.0
1	C	384	GLU	3.8
1	C	279	SER	3.8
1	G	377	ALA	3.8
1	E	208	TYR	3.7
1	G	304	TYR	3.6
1	F	383	LYS	3.6
1	E	304	TYR	3.5
1	G	280	THR	3.4
1	H	378	GLY	3.3
1	H	380	SER	3.3
1	G	384	GLU	3.2
1	B	381	SER	3.2
1	G	380	SER	3.1
1	D	382	GLY	3.1
1	E	210	LEU	3.1
1	E	136	THR	3.0
1	C	394	GLU	3.0
1	G	382	GLY	3.0
1	E	379	ILE	2.9
1	G	379	ILE	2.9
1	D	377	ALA	2.8
1	E	380	SER	2.8
1	H	379	ILE	2.8
1	B	502	ASP	2.7
1	H	484	ILE	2.7
1	C	381	SER	2.7
1	E	158	ARG	2.6
1	B	383	LYS	2.6
1	G	376	ASP	2.6
1	B	157	ILE	2.6
1	E	151	PRO	2.5
1	E	155	ASP	2.5
1	G	296	LEU	2.5
1	E	282	GLU	2.5
1	G	278	GLY	2.5
1	G	281	GLY	2.5
1	H	497	PHE	2.5
1	E	147	GLN	2.4
1	F	137	GLY	2.4
1	E	337	GLU	2.4
1	G	95	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	279	SER	2.3
1	H	384	GLU	2.3
1	F	341	ASP	2.2
1	C	339	PHE	2.1
1	B	415	ASP	2.1
1	G	85	GLU	2.1
1	F	384	GLU	2.1
1	G	282	GLU	2.1
1	G	369	LEU	2.1
1	G	390	LEU	2.1
1	G	301	TRP	2.0
1	E	279	SER	2.0
1	C	337	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	NLG	H	1503	13/13	0.91	0.27	2.82	64,81,101,106	0
2	NLG	D	1503	13/13	0.95	0.19	0.01	48,59,72,79	0

6.5 Other polymers (i)

There are no such residues in this entry.