



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:47 AM UTC

PDB ID : 4AB7 / pdb_00004ab7
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.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

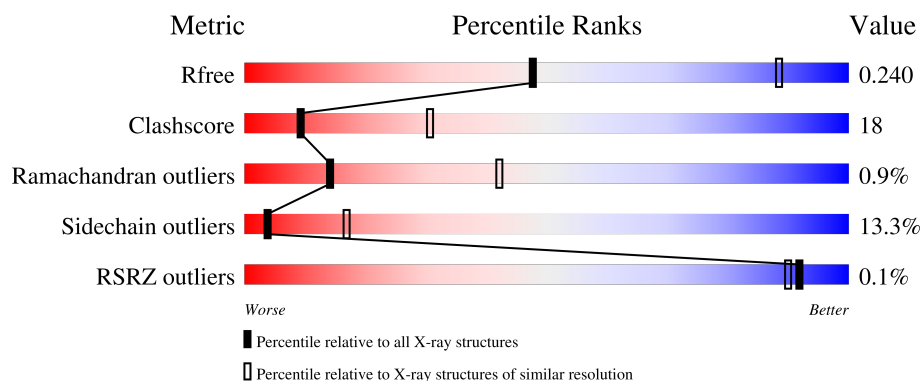
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	464	
1	B	464	
1	C	464	
1	D	464	
1	E	464	

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Mol	Chain	Length	Quality of chain
1	F	464	
1	G	464	
1	H	464	

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 Entry composition

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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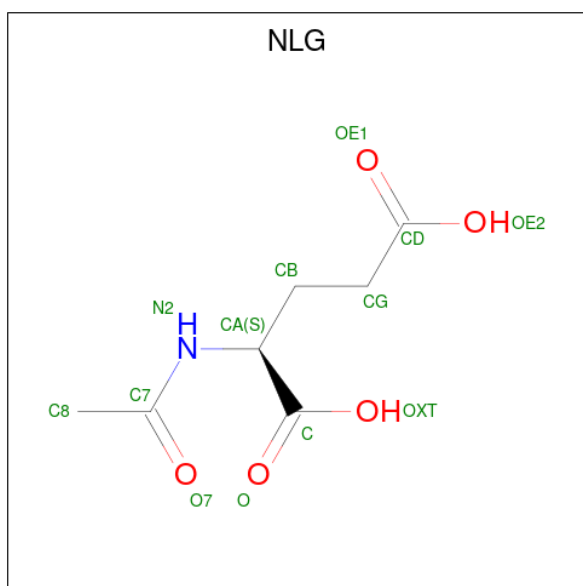
Chain	Residue	Modelled	Actual	Comment	Reference
B	55	HIS	-	expression tag	UNP Q01217
B	56	HIS	-	expression tag	UNP Q01217
B	57	HIS	-	expression tag	UNP Q01217
C	50	MET	-	expression tag	UNP Q01217
C	51	GLY	-	expression tag	UNP Q01217
C	52	HIS	-	expression tag	UNP Q01217
C	53	HIS	-	expression tag	UNP Q01217
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 (CCD ID: NLG) (formula: C₇H₁₁NO₅).

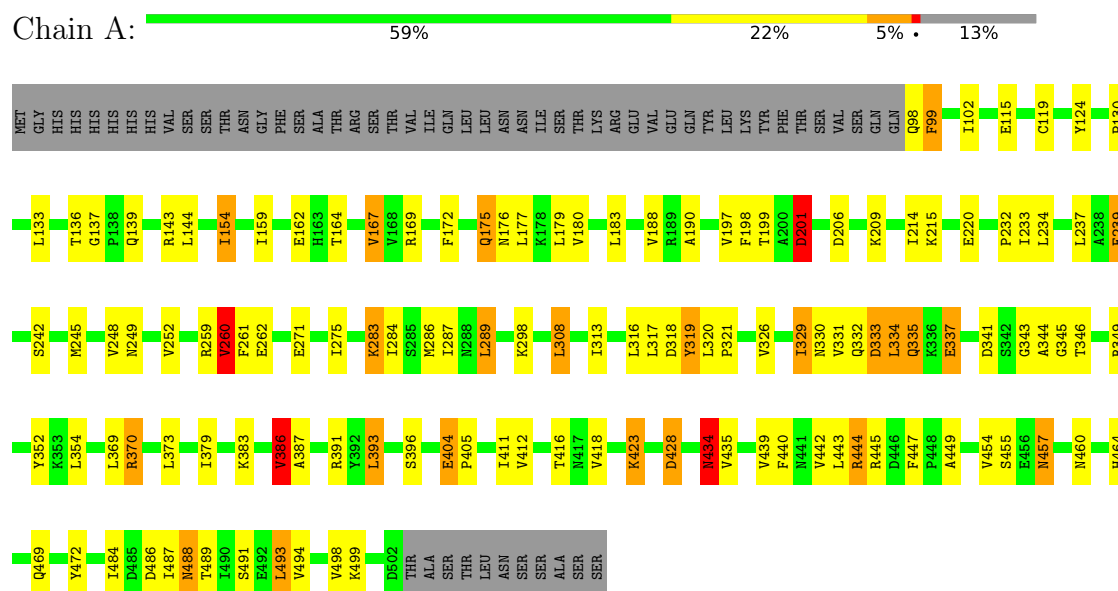


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			13	7	1	5		
2	H	1	Total	C	N	O	0	0
			13	7	1	5		

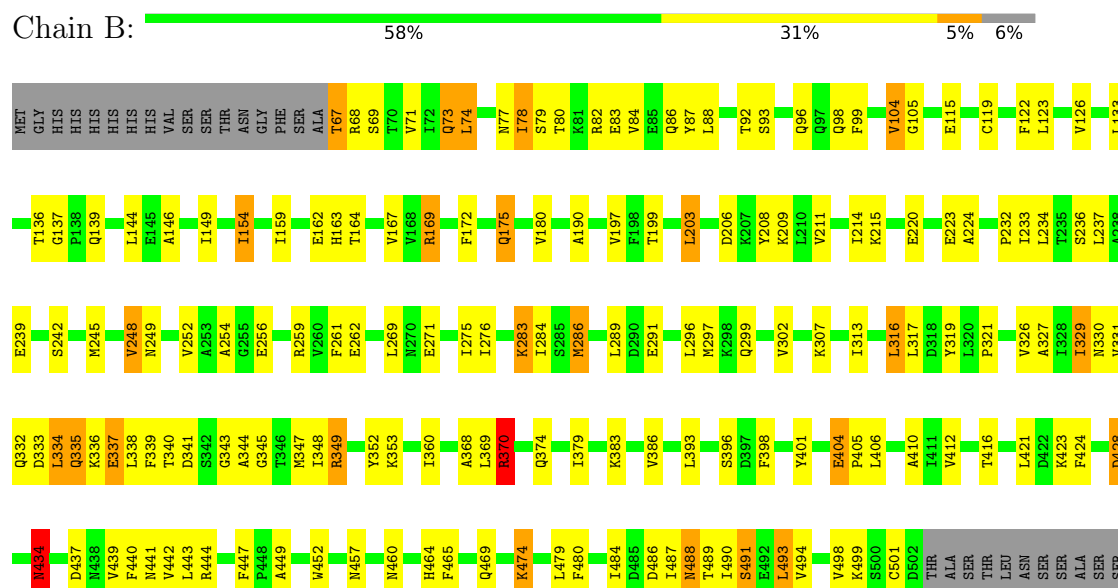
3 Residue-property plots

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

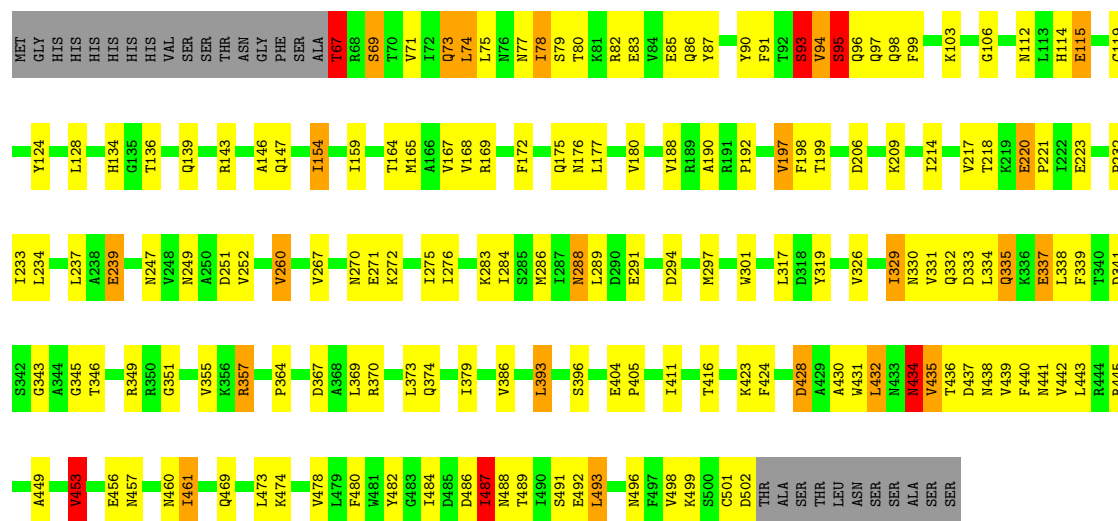


• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL



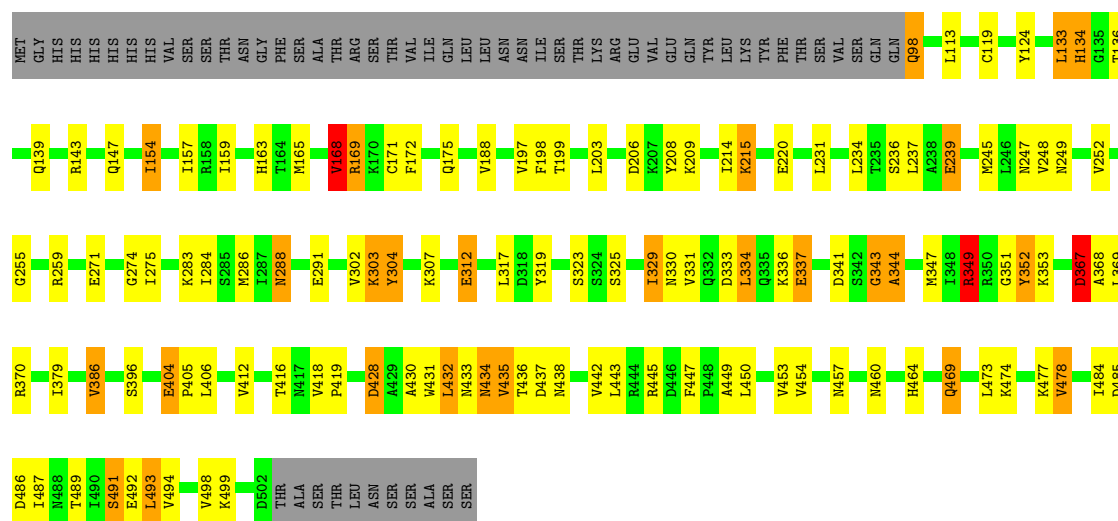
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain C:  58% 30% 5% • 6%



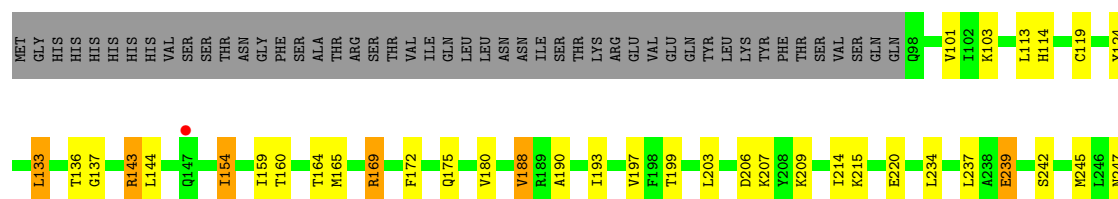
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

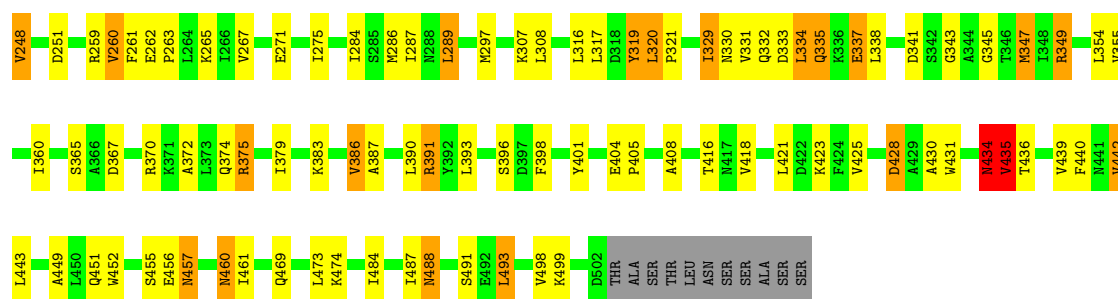
Chain D:  60% 21% 6% • 13%



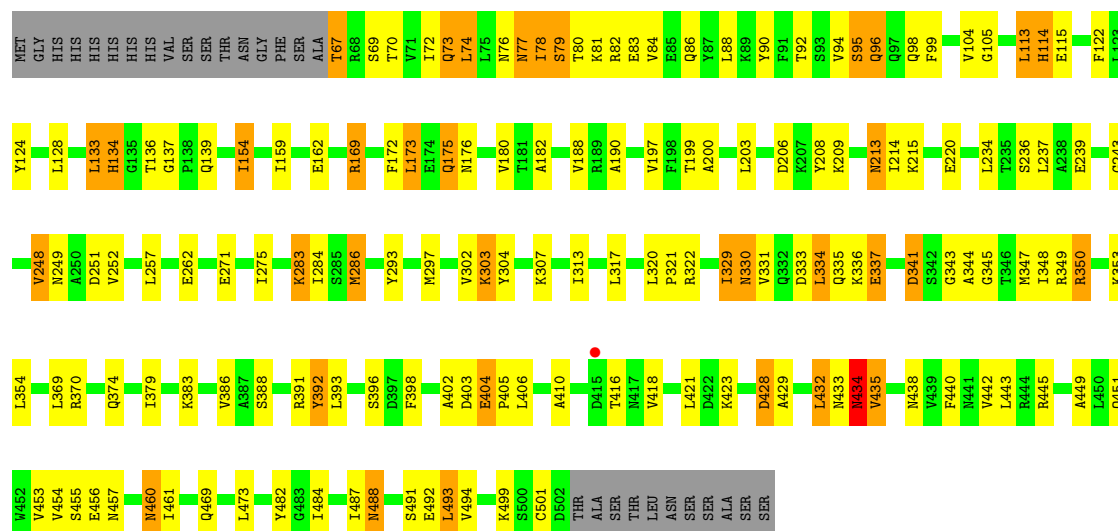
• Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain E:  59% 22% 6% 13%

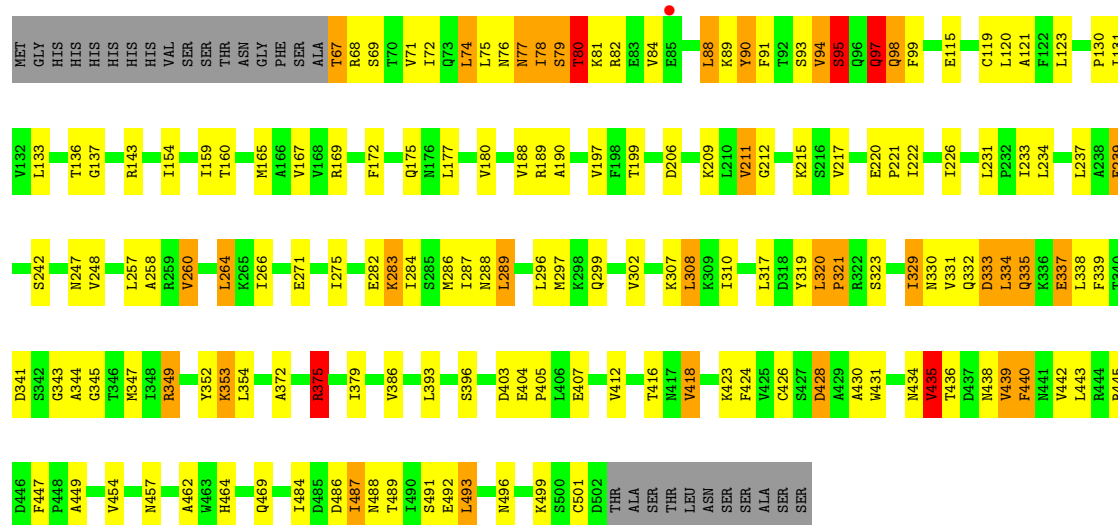




- Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL



- Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL



- Molecule 1: PROTEIN ARG5,6, MITOCHONDRIAL

Chain H: 58% 28% 5% 9%

MET	GLY	HIS	HIS	HIS	HIS	HIS	HIS	VAL	SER	SER	THR	ASN	GLY	PHE	SER	SER	ALA	THR	ARG	SER	THR	VAL	ILE	GLN	LEU	LEU	ASN	ASN	ILE	SER	THR	THR	K81	Q86	Y87	L88	K89	Y90	F91	T92	S93	V94	S95	Q96	Q97	Q98	F99	G106	L113	H114	E115	L116	A117	S118	G119	L120	A121
Y124	L133	H134	G135	T136	Q139	V140	L144	I154	D155	I159	T160	D161	E162	H163	T164	M165	V167	V168	R169	K170	C171	F172	Q175	M176	L177	V180	T181	A182	L183	E184	V188	R189	A190	R191	P192	I193	F198	T199	L203	D206	N213	T214	K215	E220	P221												
I222	L231	P232	L233	L234	T235	S236	L237	A238	E239	N247	L264	E271	G274	I275	I284	S285	N286	I287	N288	E291	E292	Y293	L296	N297	V302	K303	Y304	K307	L308	K309	I310	R311	E312	L317	L320	P321	R322	T328	I329	N330	V331	Q332	D333	L334	Q335	K336											
E337	L338	F339	D340	S341	G342	G343	A344	G345	T346	N347	T348	R349	Y352	K353	L354	R357	E362	R370	I379	K383	V386	L393	S396	A402	D403	E404	P405	L406	E407	I411	T416	P419	K423	S427	D428	A429	A430	W431	L432	W433	W434	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	I490	S491	E492	L493	V494	V498	K499	S500	C501	D502	THR	ALA	SER	THR	LEU	ASN	SER	SER	ALA	SER	SER														

4 Data and refinement statistics

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 – 3.25 108.36 – 3.25	Depositor EDS
% Data completeness (in resolution range)	96.2 (108.36-3.25) 95.6 (108.36-3.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	81.9	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.00	2/3195 (0.1%)	1.07	11/4329 (0.3%)
1	B	1.04	4/3458 (0.1%)	1.12	9/4685 (0.2%)
1	C	1.05	5/3452 (0.1%)	1.13	14/4678 (0.3%)
1	D	0.99	3/3195 (0.1%)	1.09	8/4329 (0.2%)
1	E	0.94	2/3197 (0.1%)	1.04	8/4332 (0.2%)
1	F	1.01	2/3460 (0.1%)	1.10	12/4686 (0.3%)
1	G	0.98	2/3454 (0.1%)	1.12	13/4681 (0.3%)
1	H	1.00	6/3338 (0.2%)	1.07	9/4522 (0.2%)
All	All	1.00	26/26749 (0.1%)	1.09	84/36242 (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 (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	SER	CA-C	7.18	1.62	1.52
1	E	114	HIS	CG-CD2	6.82	1.43	1.35
1	B	163	HIS	CG-CD2	6.10	1.42	1.35
1	F	134	HIS	CG-ND1	-6.04	1.31	1.38
1	D	134	HIS	CG-ND1	-5.89	1.31	1.38
1	C	134	HIS	CG-ND1	-5.79	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	ASP	CA-CB	5.78	1.62	1.53
1	G	77	ASN	N-CA	5.76	1.53	1.46
1	H	431	TRP	NE1-CE2	-5.76	1.31	1.37
1	B	67	THR	N-CA	5.75	1.57	1.46
1	F	114	HIS	CG-CD2	5.70	1.42	1.35
1	H	134	HIS	CG-CD2	5.66	1.42	1.35
1	H	328	ILE	C-O	-5.63	1.17	1.24
1	C	67	THR	N-CA	5.59	1.56	1.46
1	B	327	ALA	CA-C	-5.45	1.46	1.52
1	A	464	HIS	CG-ND1	-5.43	1.32	1.38
1	G	95	SER	CA-C	5.30	1.59	1.52
1	H	274	GLY	N-CA	-5.25	1.37	1.44
1	C	114	HIS	CA-C	-5.24	1.46	1.52
1	D	163	HIS	CA-C	-5.17	1.46	1.52
1	C	134	HIS	ND1-CE1	5.10	1.37	1.32
1	E	452	TRP	NE1-CE2	-5.10	1.31	1.37
1	D	274	GLY	N-CA	-5.08	1.37	1.44
1	H	134	HIS	CG-ND1	-5.08	1.32	1.38
1	B	464	HIS	CG-ND1	-5.05	1.32	1.38
1	H	163	HIS	CA-C	-5.03	1.46	1.52

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	375	ARG	NE-CZ-NH2	-10.84	109.45	119.20
1	D	344	ALA	N-CA-C	9.67	124.20	107.28
1	A	423	LYS	CB-CG-CD	8.39	130.59	111.30
1	C	319	TYR	CA-CB-CG	-8.21	99.13	113.90
1	H	96	GLN	N-CA-C	8.13	121.06	111.71
1	C	351	GLY	CA-C-N	-8.13	110.75	122.94
1	C	351	GLY	C-N-CA	-8.13	110.75	122.94
1	G	375	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	A	318	ASP	CA-C-N	-7.89	109.84	122.23
1	A	318	ASP	C-N-CA	-7.89	109.84	122.23
1	G	353	LYS	N-CA-C	-7.81	96.84	109.96
1	H	345	GLY	CA-C-O	-7.66	114.37	121.72
1	A	386	VAL	CB-CA-C	-7.64	102.04	112.04
1	G	90	TYR	CA-CB-CG	7.12	126.71	113.90
1	F	350	ARG	CG-CD-NE	-6.95	96.70	112.00
1	F	392	TYR	CB-CA-C	-6.90	99.33	110.79
1	D	168	VAL	CB-CA-C	-6.79	103.27	111.97
1	G	80	THR	N-CA-C	-6.61	96.55	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	291	GLU	CA-CB-CG	6.56	127.23	114.10
1	H	345	GLY	N-CA-C	-6.53	102.12	111.20
1	E	169	ARG	CA-CB-CG	-6.41	101.28	114.10
1	C	67	THR	N-CA-CB	6.39	122.37	111.50
1	B	370	ARG	CB-CG-CD	6.36	125.92	111.30
1	C	453	VAL	CB-CA-C	-6.26	101.88	110.77
1	A	260	VAL	CB-CA-C	-6.25	103.59	112.22
1	C	349	ARG	CB-CG-CD	-6.22	96.99	111.30
1	E	188	VAL	CB-CA-C	-6.09	102.55	110.84
1	F	137	GLY	CA-C-N	6.02	125.50	119.24
1	F	137	GLY	C-N-CA	6.02	125.50	119.24
1	E	391	ARG	CB-CA-C	-5.97	101.50	110.88
1	A	319	TYR	CA-CB-CG	-5.85	103.37	113.90
1	C	349	ARG	CG-CD-NE	5.83	124.83	112.00
1	H	90	TYR	CA-CB-CG	5.73	124.22	113.90
1	F	74	LEU	N-CA-C	-5.72	104.73	110.97
1	E	319	TYR	CA-CB-CG	5.69	124.14	113.90
1	G	319	TYR	CA-CB-CG	5.65	124.08	113.90
1	A	99	PHE	N-CA-C	5.65	119.79	111.04
1	C	74	LEU	N-CA-C	-5.64	104.82	110.97
1	B	137	GLY	CA-C-N	5.62	125.08	119.24
1	B	137	GLY	C-N-CA	5.62	125.08	119.24
1	G	74	LEU	N-CA-C	-5.61	104.86	110.97
1	B	74	LEU	N-CA-C	-5.58	104.89	110.97
1	H	501	CYS	N-CA-C	5.57	118.89	107.69
1	G	435	VAL	N-CA-C	-5.51	104.06	111.44
1	H	438	ASN	CB-CA-C	-5.51	102.16	110.92
1	F	492	GLU	CG-CD-OE1	-5.46	105.84	118.40
1	A	318	ASP	CA-C-O	5.45	126.09	119.49
1	H	352	TYR	N-CA-C	-5.45	101.02	109.14
1	C	438	ASN	CB-CA-C	-5.43	102.12	110.81
1	H	354	LEU	N-CA-C	-5.42	102.45	110.48
1	G	137	GLY	CA-C-N	5.40	124.86	119.24
1	G	137	GLY	C-N-CA	5.40	124.86	119.24
1	F	501	CYS	N-CA-C	-5.39	99.33	110.80
1	A	167	VAL	CB-CA-C	-5.38	104.80	112.22
1	B	349	ARG	CD-NE-CZ	-5.36	116.89	124.40
1	F	453	VAL	N-CA-C	5.35	115.68	107.77
1	E	137	GLY	CA-C-N	5.31	124.77	119.24
1	E	137	GLY	C-N-CA	5.31	124.77	119.24
1	A	137	GLY	CA-C-N	5.31	124.76	119.24
1	A	137	GLY	C-N-CA	5.31	124.76	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	349	ARG	CG-CD-NE	-5.30	100.33	112.00
1	F	438	ASN	CB-CA-C	-5.30	102.34	110.81
1	B	104	VAL	CB-CA-C	-5.28	103.25	110.96
1	E	355	VAL	CB-CA-C	-5.28	103.27	110.77
1	G	167	VAL	CB-CA-C	-5.25	104.97	112.22
1	G	501	CYS	N-CA-C	-5.24	99.64	110.80
1	D	215	LYS	CB-CG-CD	5.22	123.30	111.30
1	F	213	ASN	CA-CB-CG	5.22	117.82	112.60
1	C	96	GLN	N-CA-C	5.21	119.97	111.37
1	B	122	PHE	CA-CB-CG	5.20	119.00	113.80
1	G	211	VAL	CB-CA-C	-5.20	103.65	110.98
1	D	343	GLY	CA-C-N	-5.19	113.53	121.26
1	D	343	GLY	C-N-CA	-5.19	113.53	121.26
1	E	435	VAL	N-CA-C	-5.15	104.54	111.44
1	D	367	ASP	N-CA-CB	5.15	117.69	110.12
1	F	492	GLU	CG-CD-OE2	5.14	130.23	118.40
1	C	453	VAL	N-CA-C	5.14	115.26	107.75
1	C	94	VAL	N-CA-C	-5.11	104.89	112.04
1	D	453	VAL	N-CA-C	5.08	115.23	108.11
1	C	435	VAL	N-CA-C	-5.08	104.64	111.44
1	B	352	TYR	N-CA-C	-5.05	101.61	109.24
1	F	336	LYS	CB-CG-CD	5.05	122.91	111.30
1	C	294	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	99	PHE	N-CA-C	5.03	117.73	111.24

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

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	103	1
1	B	3400	0	3418	143	0
1	C	3394	0	3407	132	1
1	D	3140	0	3153	120	0
1	E	3142	0	3153	117	1
1	F	3402	0	3429	156	1
1	G	3396	0	3407	157	1
1	H	3280	0	3286	106	1
2	D	13	0	9	10	0
2	H	13	0	9	2	0
All	All	26320	0	26424	956	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 18.

All (956) 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
1:B:474:LYS:HD2	1:B:474:LYS:O	1.43	1.18
1:C:379:ILE:HG21	1:C:386:VAL:HG23	1.24	1.18
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:HE2	1:D:438:ASN:ND2	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:474:LYS:HD2	1:B:474:LYS:C	1.90	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:F:286:MET:HE2	1:F:434:ASN:ND2	1.83	0.93
1:A:387:ALA:HB2	1:E:262:GLU:CD	1.94	0.93
1:F:379:ILE:CG2	1:F:386:VAL:HG23	1.99	0.93
1:E:379:ILE:HD11	1:E:423:LYS:HZ3	1.20	0.93
2:D:1503:NLG:H8C1	2:D:1503:NLG:CB	1.98	0.92
1:D:286:MET:CE	1:D:438:ASN:ND2	2.31	0.92
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:E:379:ILE:HD11	1:E:423:LYS:HZ2	1.35	0.91
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:286:MET:HE2	1:D:438:ASN:HD22	1.31	0.89
1:C:297:MET:HE2	1:C:297:MET:HA	1.53	0.89
1:D:154:ILE:HG13	1:D:159:ILE:HD11	1.53	0.89
1:B:474:LYS:C	1:B:474:LYS:CD	2.46	0.89
1:F:379:ILE:HD11	1:F:423:LYS:CE	2.03	0.88
1:E:143:ARG:HG3	1:E:143:ARG:HH11	1.38	0.88
1:F:80:THR:HG22	1:F:82:ARG:N	1.87	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:ALA:HB1	1:D:435:VAL:HG21	1.56	0.88
1:B:297:MET:HE1	1:B:307:LYS:CB	2.05	0.87
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: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: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:D:286:MET:CE	1:D:438:ASN:HD21	1.88	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
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:H:160:THR:HG21	1:H:165:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:291:GLU:HG2	1:H:353:LYS:HE3	1.62	0.79
1:C:67:THR:HG21	1:C:69:SER:OG	1.83	0.79
1:C:197:VAL:HG21	1:C:234:LEU:HD11	1.64	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:H:165:MET:HE1	1:H:247:ASN:HB2	1.66	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: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:D:239:GLU:OE1	1:D:245:MET:HE3	1.85	0.77
1:F:484:ILE:HD11	1:F:493:LEU:HD22	1.66	0.77
1:D:255:GLY:HA3	1:D:312:GLU:OE2	1.85	0.77
2:D:1503:NLG:H8C1	2:D:1503:NLG:HBC1	1.65	0.77
1:B:474:LYS:NZ	1:B:501:CYS:SG	2.57	0.77
1:D:248:VAL:C	2:D:1503:NLG:H8C3	2.10	0.76
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: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
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:F:136:THR:HG23	1:F:136:THR:O	1.87	0.73
1:C:453:VAL:O	1:C:453:VAL:CG1	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:B:474:LYS:O	1:B:474:LYS:CD	2.31	0.73
1:C:276:ILE:CD1	1:C:283:LYS:CD	2.66	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:237:LEU:HD23	1:E:245:MET:HE1	1.69	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:G:136:THR:O	1:G:136:THR:HG23	1.89	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:G:160:THR:HG21	1:G:165:MET:HE2	1.70	0.72
1:D:430:ALA:O	1:D:435:VAL:HG13	1.90	0.72
1:G:80:THR:O	1:G:80:THR:HG22	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: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:E:239:GLU:HG3	1:F:169:ARG:NH2	2.06	0.71
1:G:74:LEU:C	1:G:74:LEU:HD23	2.15	0.71
1:F:90:TYR:HE2	1:F:128:LEU:CD1	2.04	0.71
1:F:283:LYS:HZ2	1:F:344:ALA:HA	1.55	0.71
1:F:293:TYR:OH	1:F:297:MET:HE2	1.90	0.70
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
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:D:286:MET:HE1	1:D:438:ASN:HD21	1.55	0.69
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:C:67:THR:HG22	1:C:69:SER:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:ARG:CG	1:E:386:VAL:HG11	2.23	0.69
1:F:329:ILE:HG22	1:F:345:GLY:HA3	1.75	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:D:248:VAL:C	2:D:1503:NLG:C8	2.66	0.68
1:E:275:ILE:HG22	1:E:284:ILE:HD12	1.75	0.68
1:G:160:THR:CG2	1:G:165:MET:HE2	2.24	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:HG12	1:E:425:VAL:O	1.94	0.67
1:G:97:GLN:OE1	1:G:98:GLN:N	2.28	0.67
1:G:297:MET:HE1	1:G:307:LYS:CB	2.23	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:B:488:ASN:C	1:B:488:ASN:HD22	2.03	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:67:THR:CG2	1:C:69:SER:OG	2.43	0.67
1:C:154:ILE:CG1	1:C:159:ILE:HD11	2.25	0.67
1:F:402:ALA:HB1	1:F:406:LEU:HD23	1.77	0.67
1:F:286:MET:HE2	1:F:434:ASN:CG	2.18	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:C:430:ALA:HB1	1:C:435:VAL:CG2	2.26	0.66
1:D:352:TYR:HH	1:D:435:VAL:HG12	1.59	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
1:C:317:LEU:HD21	1:C:326:VAL:HG23	1.78	0.66
1:F:88:LEU:HD21	1:G:76:ASN:ND2	2.10	0.66
1:F:173:LEU:N	1:F:173:LEU:HD23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:262:GLU:OE2	1:E:387:ALA:HB2	1.97	0.65
1:C:180:VAL:HG13	1:C:190:ALA:HB3	1.78	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:286:MET:CE	1:F:434:ASN:ND2	2.59	0.64
1:F:449:ALA:HB1	1:F:484:ILE:HG23	1.80	0.64
1:B:474:LYS:HE2	1:B:501:CYS:HG	1.55	0.64
1:A:449:ALA:HB1	1:A:484:ILE:HG23	1.79	0.64
1:E:169:ARG:NH2	1:F:239:GLU:OE2	2.30	0.64
1:F:176:ASN:O	1:F:180:VAL:HG23	1.96	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:G:286:MET:HE3	1:G:287:ILE:N	2.13	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:F:72:ILE:C	1:G:89:LYS:NZ	2.53	0.63
1:C:147:GLN:HE22	1:C:167:VAL:HG22	1.63	0.63
1:G:286:MET:HE2	1:G:288:ASN:OD1	1.98	0.63
1:B:286:MET:HE2	1:B:347:MET:HE3	1.81	0.62
1:G:426:CYS:HG	1:G:431:TRP:CD1	2.17	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: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
1:H:172:PHE:CD2	1:H:237:LEU:HD13	2.35	0.62
1:H:308:LEU:HD12	1:H:308:LEU:O	1.98	0.62
1:C:99:PHE:CZ	1:C:338:LEU:HD13	2.35	0.62
1:F:286:MET:CG	1:F:434:ASN:ND2	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:432:LEU:N	1:H:432:LEU:HD23	2.15	0.62
1:A:172:PHE:CE2	1:A:237:LEU:HD13	2.34	0.61
1:A:197:VAL:HG21	1:A:234:LEU:HD11	1.80	0.61
1:B:77:ASN:OD1	1:B:335:GLN:OE1	2.18	0.61
1:E:136:THR:HG23	1:E:136:THR:O	1.99	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:172:PHE:CD2	1:G:237:LEU:HD13	2.35	0.61
1:G:180:VAL:HG13	1:G:190:ALA:HB3	1.83	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:O	1:B:136:THR:HG23	2.01	0.60
1:F:74:LEU:HD21	1:F:78:ILE:HD11	1.83	0.60
1:G:97:GLN:C	1:G:99:PHE:H	2.09	0.60
1:B:283:LYS:NZ	1:B:344:ALA:CA	2.63	0.60
1:E:160:THR:HG21	1:E:165:MET:HE2	1.82	0.60
1:H:442:VAL:HG13	1:H:445:ARG:NH1	2.15	0.60
1:D:139:GLN:H	1:D:139:GLN:CD	2.10	0.60
2:D:1503:NLG:H8C1	2:D:1503:NLG:HBC2	1.82	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:G:286:MET:HE1	1:G:288:ASN:OD1	2.02	0.59
1:H:288:ASN:ND2	1:H:438:ASN:HD21	2.00	0.59
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:H:302:VAL:HG12	1:H:307:LYS:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:293:TYR:CE1	1:H:297:MET:HE2	2.37	0.58
1:B:172:PHE:CD2	1:B:237:LEU:HD13	2.37	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:80:THR:CG2	1:F:82:ARG:H	2.05	0.58
1:F:133:LEU:C	1:F:133:LEU:CD2	2.77	0.58
1:F:302:VAL:HG12	1:F:307:LYS:HG3	1.86	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: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:D:165:MET:HE1	1:D:247:ASN:N	2.20	0.57
1:E:297:MET:HE1	1:E:307:LYS:CB	2.34	0.57
1:E:330:ASN:OD1	1:E:331:VAL:N	2.37	0.57
1:F:79:SER:HA	1:G:82:ARG:HD3	1.86	0.57
1:F:173:LEU:N	1:F:173:LEU:CD2	2.68	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:297:MET:HE2	1:H:310:ILE:HG22	1.87	0.57
1:A:317:LEU:HA	1:A:320:LEU:HD12	1.87	0.56
1:G:160:THR:HG21	1:G:165:MET:CE	2.35	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:E:265:LYS:NZ	1:E:347:MET:HE1	2.20	0.56
1:F:124:TYR:CD2	1:F:188:VAL:HG13	2.40	0.56
1:H:198:PHE:CD1	1:H:214:ILE:HD13	2.39	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:N	1:F:77:ASN:HD22	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:A:386:VAL:HG12	1:A:387:ALA:N	2.15	0.56
1:A:404:GLU:CD	1:E:365:SER:OG	2.49	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:333:ASP:OD1	1:G:333:ASP:N	2.39	0.56
1:C:424:PHE:HE1	1:C:439:VAL:HG11	1.70	0.56
1:F:77:ASN:N	1:F:77:ASN:ND2	2.53	0.56
1:F:197:VAL:HG21	1:F:234:LEU:HD11	1.87	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: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
1:D:418:VAL:HG11	1:D:493:LEU:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:133:LEU:C	1:H:133:LEU:CD2	2.80	0.55
1:D:352:TYR:CD1	1:D:352:TYR:N	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:B:169:ARG:NH1	1:B:245:MET:HE3	2.23	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:D:247:ASN:CG	2:D:1503:NLG:H8C2	2.33	0.54
1:E:372:ALA:O	1:E:375:ARG:HD2	2.09	0.54
1:F:133:LEU:C	1:F:133:LEU:HD23	2.32	0.54
1:F:172:PHE:CD2	1:F:237:LEU:CD1	2.91	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:C:106:GLY:C	1:C:139:GLN:HE22	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:457:ASN:C	1:H:457:ASN:HD22	2.16	0.53
1:A:172:PHE:CD2	1:A:237:LEU:HD13	2.44	0.53
1:A:472:TYR:OH	1:D:485:ASP:HB2	2.09	0.53
1:G:353:LYS:O	1:G:354:LEU:HD23	2.08	0.53
1:B:248:VAL:HG12	1:B:248:VAL:O	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:F:293:TYR:CZ	1:F:297:MET:HE2	2.44	0.53
1:C:428:ASP:OD1	1:C:428:ASP:N	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:325:SER:HB2	1:D:347:MET:HE2	1.92	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:B:154:ILE:CG1	1:B:159:ILE:HD11	2.38	0.52
1:D:147:GLN:HA	1:G:321:PRO:HB3	1.90	0.52
1:D:449:ALA:HB1	1:D:484:ILE:HG23	1.91	0.52
1:F:334:LEU:C	1:F:334:LEU:CD2	2.83	0.52
1:H:334:LEU:C	1:H:334:LEU:CD2	2.81	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:E:379:ILE:CD1	1:E:423:LYS:HZ3	2.08	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:H:293:TYR:HE1	1:H:297:MET:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:379:ILE:HD11	1:C:423:LYS:HZ3	1.75	0.51
1:E:457:ASN:C	1:E:457:ASN:HD22	2.19	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
1:G:79:SER:C	1:G:81:LYS:N	2.68	0.51
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:F:98:GLN:CD	1:F:99:PHE:H	2.18	0.51
1:G:74:LEU:O	1:G:77:ASN:HB2	2.10	0.51
1:H:99:PHE:HZ	1:H:338:LEU:HD13	1.76	0.51
1:H:136:THR:H	2:H:1503:NLG:HGC2	1.75	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:74:LEU:C	1:G:74:LEU:CD2	2.84	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:A:457:ASN:HD22	1:A:457:ASN:C	2.19	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:133:LEU:CD2	1:D:133:LEU:C	2.84	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:A:239:GLU:OE1	1:A:245:MET:HE3	2.10	0.50
1:F:74:LEU:HD13	1:G:71:VAL:HG13	1.92	0.50
1:B:98:GLN:CD	1:B:98:GLN:H	2.18	0.50
1:A:428:ASP:OD1	1:A:428:ASP:N	2.42	0.50
1:C:297:MET:HA	1:C:297:MET:CE	2.33	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:F:94:VAL:O	1:F:95:SER:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:133:LEU:HD13	1:A:133:LEU:C	2.36	0.49
1:A:387:ALA:CA	1:E:262:GLU:OE2	2.59	0.49
1:F:86:GLN:CG	1:F:432:LEU:HD13	2.41	0.49
1:F:275:ILE:HG22	1:F:284:ILE:HD12	1.93	0.49
1:H:106:GLY:C	1:H:139:GLN:HE22	2.20	0.49
1:H:116:LEU:CD2	1:H:120:LEU:CD1	2.90	0.49
1:H:297:MET:HE2	1:H:310:ILE:CG2	2.42	0.49
1:E:408:ALA:HB2	1:E:435:VAL:HG21	1.94	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
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:OD1	1:H:434:ASN:N	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:341:ASP:HB2	1:F:434:ASN:CG	2.37	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: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: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:HG3	1:E:143:ARG:NH1	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:D:139:GLN:HG2	1:D:175:GLN:CD	2.37	0.48
1:E:360:ILE:HD11	1:E:393:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:387:ALA:HB1	1:E:259:ARG:O	2.13	0.48
1:C:434:ASN:N	1:C:434:ASN:OD1	2.46	0.48
1:E:286:MET:HE1	1:E:349:ARG:HH11	1.78	0.48
1:E:418:VAL:HG11	1:E:493:LEU:HD21	1.95	0.48
1:F:88:LEU:HD11	1:G:76:ASN:HD22	1.77	0.48
1:F:418:VAL:CG2	1:F:484:ILE:HD13	2.43	0.48
1:C:488:ASN:C	1:C:488:ASN:HD22	2.21	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: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:E:160:THR:CG2	1:E:165:MET:HE2	2.44	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
1:H:90:TYR:OH	1:H:264:LEU:HD22	2.14	0.48
2:H:1503:NLG:OXT	2:H:1503:NLG:HGC1	2.13	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:OD1	1:F:434:ASN:N	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: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: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:94:VAL:O	1:F:96:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:GLN:HG2	1:F:175:GLN:NE2	2.30	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:A:334:LEU:C	1:A:334:LEU:CD2	2.88	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:B:299:GLN:HB2	1:B:302:VAL:HG12	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: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
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: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:265:LYS:HZ3	1:E:347:MET:HE1	1.79	0.47
1:E:287:ILE:HG22	1:E:289:LEU:HD13	1.96	0.47
1:G:79:SER:OG	1:G:81:LYS:HG3	2.15	0.47
1:A:444:ARG:HH11	1:A:444:ARG:HG2	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:F:136:THR:O	1:F:136:THR:CG2	2.59	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:133:LEU:C	1:H:133:LEU:HD23	2.41	0.46
1:H:203:LEU:HD12	1:H:203:LEU:O	2.15	0.46
1:F:432:LEU:N	1:F:432:LEU:HD23	2.31	0.46
1:C:232:PRO:C	1:C:233:ILE:HD13	2.39	0.46
1:C:357:ARG:NH2	1:C:364:PRO:HD3	2.31	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:G:95:SER:CB	1:G:98:GLN:HB2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:72:ILE:CA	1:G:89:LYS:HZ2	2.29	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: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:249:ASN:HB3	1:D:252:VAL:HG23	1.98	0.46
1:F:341:ASP:HA	1:F:347:MET:HE1	1.96	0.46
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: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:334:LEU:C	1:A:334:LEU:HD23	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:488:ASN:C	1:F:488:ASN:HD22	2.25	0.45
1:G:211:VAL:CG1	1:G:212:GLY:N	2.79	0.45
1:A:139:GLN:HE21	1:A:175:GLN:CD	2.24	0.45
1:A:434:ASN:OD1	1:A:434:ASN:N	2.49	0.45
1:D:351:GLY:C	1:D:352:TYR:CD1	2.94	0.45
1:G:84:VAL:HG13	1:G:339:PHE:HB3	1.99	0.45
1:G:97:GLN:C	1:G:99:PHE:N	2.72	0.45
1:D:147:GLN:CG	1:G:321:PRO:HG3	2.46	0.45
1:D:370:ARG:CG	1:D:386:VAL:HG11	2.35	0.45
1:E:165:MET:HE1	1:E:247:ASN:HB2	1.99	0.45
1:B:169:ARG:NH1	1:B:245:MET:CE	2.80	0.45
1:C:86:GLN:O	1:C:90:TYR:HD2	2.00	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: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:C:165:MET:HE1	1:C:247:ASN:N	2.32	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: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:C:337:GLU:HG2	1:C:343:GLY:HA3	1.99	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:A:404:GLU:OE2	1:E:367:ASP:HB3	2.17	0.44
1:B:71:VAL:HG13	1:C:74:LEU:CD2	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:354:LEU:HD23	1:H:354:LEU:HA	1.68	0.44
1:A:391:ARG:HA	1:E:319:TYR:CE2	2.53	0.44
1:D:474:LYS:HD3	1:D:498:VAL:HG13	1.98	0.44
1:G:165:MET:HE1	1:G:247:ASN:HB2	1.99	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: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
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:A:308:LEU:HD12	1:A:308:LEU:C	2.42	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:D:133:LEU:HD23	1:D:133:LEU:C	2.42	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:F:72:ILE:HA	1:G:89:LYS:HZ2	1.83	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:HE21	1:H:335:GLN:N	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:283:LYS:NZ	1:B:344:ALA:C	2.76	0.43
1:B:379:ILE:HG21	1:B:386:VAL:HG22	1.84	0.43
1:C:139:GLN:CD	1:C:139:GLN:H	2.25	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:D:432:LEU:N	1:D:432:LEU:HD23	2.33	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:LEU:CD1	1:G:71:VAL:HG13	2.48	0.43
1:F:392:TYR:O	1:F:392:TYR:CD1	2.72	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:OD1	1:F:428:ASP:N	2.42	0.43
1:G:90:TYR:OH	1:G:323:SER:CB	2.65	0.43
1:G:93:SER:O	1:G:94:VAL:CG2	2.66	0.43
1:G:349:ARG:HH11	1:G:349:ARG:HB2	1.82	0.43
1:A:239:GLU:CD	1:B:169:ARG:HH12	2.26	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
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:88:LEU:HD23	1:H:88:LEU:HA	1.74	0.43
1:H:317:LEU:HD13	1:H:349:ARG:HA	2.01	0.43
1:B:169:ARG:HH11	1:B:245:MET:CE	2.31	0.43
1:B:223:GLU:O	1:B:224:ALA:C	2.61	0.43
1:B:401:TYR:CE2	1:B:442:VAL:CG1	3.02	0.43
1:C:94:VAL:O	1:C:95:SER:C	2.61	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:E:239:GLU:OE1	1:E:245:MET:HE3	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:94:VAL:CG2	1:C:98:GLN:OE1	2.65	0.43
1:C:367:ASP:HA	1:C:370:ARG:HH12	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:160:THR:CG2	1:H:165:MET:HE2	2.39	0.43
1:H:428:ASP:O	1:H:429:ALA:C	2.61	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:C:286:MET:HE1	1:C:288:ASN:OD1	2.18	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:B:139:GLN:HE21	1:B:175:GLN:CD	2.27	0.42
1:D:147:GLN:HA	1:G:321:PRO:CB	2.50	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:A:370:ARG:CZ	1:E:321:PRO:HG3	2.48	0.42
1:D:491:SER:O	1:D:492:GLU:C	2.63	0.42
1:E:101:VAL:HG23	1:E:263:PRO:HG3	2.01	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
1:F:82:ARG:HD3	1:F:460:ASN:HD22	1.84	0.42
1:G:95:SER:HB3	1:G:98:GLN:CB	2.48	0.42
1:G:264:LEU:HD22	1:G:323:SER:OG	2.19	0.42
1:H:456:GLU:OE2	1:H:473:LEU:HD21	2.19	0.42
1:B:84:VAL:HG13	1:C:75:LEU:HD22	2.01	0.42
1:B:261:PHE:O	1:B:262:GLU:C	2.63	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: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: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:E:113:LEU:HD12	1:E:113:LEU:HA	1.77	0.42
1:F:203:LEU:HD23	1:F:208:TYR:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:488:ASN:C	1:E:488:ASN:HD22	2.28	0.42
1:G:403:ASP:OD1	1:G:403:ASP:N	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
1:E:286:MET:HE1	1:E:349:ARG:NH1	2.34	0.42
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: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:B:334:LEU:C	1:B:334:LEU:CD2	2.92	0.41
1:F:442:VAL:HG13	1:F:445:ARG:HH11	1.84	0.41
1:H:457:ASN:O	1:H:457:ASN:ND2	2.46	0.41
1:C:93:SER:CB	1:C:95:SER:H	2.33	0.41
1:C:218:THR:HG22	1:C:220:GLU:HG2	2.01	0.41
1:D:433:ASN:O	1:D:434:ASN:C	2.62	0.41
1:E:193:ILE:HB	1:E:234:LEU:HD13	2.02	0.41
1:F:94:VAL:O	1:F:94:VAL:CG1	2.67	0.41
1:A:354:LEU:HA	1:A:354:LEU:HD23	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:E:133:LEU:HD13	1:E:133:LEU:C	2.45	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:B:169:ARG:HH11	1:B:245:MET:HE1	1.86	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:O	1:G:136:THR:CG2	2.60	0.41
1:G:189:ARG:HH12	1:H:184:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:165:MET:HE1	1:H:247:ASN:N	2.35	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:HA	1:B:296:LEU:HD12	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:E:103:LYS:NZ	1:E:251:ASP:OD1	2.52	0.41
1:F:494:VAL:CG1	1:G:487:ILE:HD12	2.50	0.41
1:G:430:ALA:HA	1:G:435:VAL:CG1	2.51	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:F:428:ASP:O	1:F:429:ALA:C	2.63	0.41
1:B:434:ASN:OD1	1:B:434:ASN:N	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:D:334:LEU:C	1:D:334:LEU:CD2	2.94	0.41
1:F:67:THR:N	1:G:67:THR:HG22	2.35	0.41
1:F:454:VAL:HG12	1:F:455:SER:N	2.36	0.41
1:H:334:LEU:C	1:H:334:LEU:HD23	2.45	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
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:A:283:LYS:HZ1	1:A:345:GLY:N	2.19	0.41
1:D:412:VAL:HG11	1:D:447:PHE:CZ	2.56	0.41
1:E:451:GLN:NE2	1:E:493:LEU:HD11	2.36	0.41
1:E:455:SER:O	1:E:461:ILE:HD13	2.21	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: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: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:A:352:TYR:CD2	1:A:352:TYR:C	2.99	0.40
1:B:368:ALA:CB	1:B:406:LEU:HD13	2.48	0.40
1:E:337:GLU:OE1	1:E:347:MET:HE3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	1:C:461:ILE:O	2.21	0.40
1:E:347:MET:HE3	1:E:347:MET:HB2	1.83	0.40
1:F:403:ASP:OD1	1:F:403:ASP:N	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:A:201:ASP:OD1	1:A:201:ASP:N	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:C:482:TYR:C	1:C:482:TYR:CD1	2.99	0.40
1:D:203:LEU:HD23	1:D:208:TYR:CE2	2.56	0.40
1:D:418:VAL:HG21	1:D:484:ILE:CD1	2.49	0.40
1:F:482:TYR:CD1	1:F:482:TYR:C	3.00	0.40
1:G:257:LEU:HD23	1:G:257:LEU:HA	1.85	0.40
1:H:155:ASP:HA	1:H:304:TYR:CE2	2.57	0.40
1:A:393:LEU:HD11	1:A:411:ILE:HD13	2.02	0.40
1:B:86:GLN:CD	1:B:339:PHE:O	2.65	0.40
1:C:103:LYS:NZ	1:C:251:ASP:OD1	2.44	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:HA	1:C:237:LEU:HD12	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	403/464 (87%)	371 (92%)	29 (7%)	3 (1%)	18	48
1	B	434/464 (94%)	397 (92%)	32 (7%)	5 (1%)	10	36
1	C	434/464 (94%)	397 (92%)	33 (8%)	4 (1%)	14	42
1	D	403/464 (87%)	370 (92%)	31 (8%)	2 (0%)	24	55
1	E	403/464 (87%)	369 (92%)	31 (8%)	3 (1%)	18	48
1	F	434/464 (94%)	395 (91%)	36 (8%)	3 (1%)	18	48
1	G	434/464 (94%)	392 (90%)	36 (8%)	6 (1%)	9	33
1	H	420/464 (90%)	386 (92%)	30 (7%)	4 (1%)	12	40
All	All	3365/3712 (91%)	3077 (91%)	258 (8%)	30 (1%)	14	42

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

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Mol	Chain	Res	Type
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 ⓘ

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%)	293 (86%)	47 (14%)	3	15
1	B	371/397 (94%)	321 (86%)	50 (14%)	4	16
1	C	370/397 (93%)	324 (88%)	46 (12%)	4	19
1	D	340/397 (86%)	297 (87%)	43 (13%)	4	19
1	E	340/397 (86%)	298 (88%)	42 (12%)	4	19
1	F	372/397 (94%)	323 (87%)	49 (13%)	4	17
1	G	370/397 (93%)	318 (86%)	52 (14%)	3	15
1	H	355/397 (89%)	305 (86%)	50 (14%)	3	15
All	All	2858/3176 (90%)	2479 (87%)	379 (13%)	4	17

All (379) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	GLU
1	A	143	ARG

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Mol	Chain	Res	Type
1	A	154	ILE
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	248	VAL
1	A	260	VAL
1	A	271	GLU
1	A	283	LYS
1	A	286	MET
1	A	289	LEU
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	337	GLU
1	A	341	ASP
1	A	349	ARG
1	A	370	ARG
1	A	383	LYS
1	A	386	VAL
1	A	393	LEU
1	A	396	SER
1	A	404	GLU
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

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Mol	Chain	Res	Type
1	A	491	SER
1	A	493	LEU
1	A	499	LYS
1	B	67	THR
1	B	69	SER
1	B	73	GLN
1	B	78	ILE
1	B	79	SER
1	B	80	THR
1	B	82	ARG
1	B	88	LEU
1	B	115	GLU
1	B	154	ILE
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	248	VAL
1	B	256	GLU
1	B	271	GLU
1	B	283	LYS
1	B	286	MET
1	B	289	LEU
1	B	316	LEU
1	B	329	ILE
1	B	333	ASP
1	B	334	LEU
1	B	335	GLN
1	B	337	GLU
1	B	341	ASP
1	B	349	ARG
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

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Mol	Chain	Res	Type
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	493	LEU
1	B	499	LYS
1	C	67	THR
1	C	69	SER
1	C	73	GLN
1	C	78	ILE
1	C	79	SER
1	C	80	THR
1	C	82	ARG
1	C	93	SER
1	C	95	SER
1	C	115	GLU
1	C	143	ARG
1	C	154	ILE
1	C	175	GLN
1	C	177	LEU
1	C	197	VAL
1	C	199	THR
1	C	206	ASP
1	C	209	LYS
1	C	220	GLU
1	C	239	GLU
1	C	260	VAL
1	C	271	GLU
1	C	288	ASN
1	C	289	LEU
1	C	329	ILE
1	C	333	ASP
1	C	335	GLN
1	C	337	GLU
1	C	341	ASP
1	C	357	ARG
1	C	393	LEU

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Mol	Chain	Res	Type
1	C	396	SER
1	C	428	ASP
1	C	432	LEU
1	C	434	ASN
1	C	440	PHE
1	C	443	LEU
1	C	453	VAL
1	C	457	ASN
1	C	460	ASN
1	C	461	ILE
1	C	469	GLN
1	C	487	ILE
1	C	491	SER
1	C	493	LEU
1	C	499	LYS
1	D	98	GLN
1	D	113	LEU
1	D	133	LEU
1	D	143	ARG
1	D	154	ILE
1	D	168	VAL
1	D	169	ARG
1	D	199	THR
1	D	206	ASP
1	D	209	LYS
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	303	LYS
1	D	304	TYR
1	D	312	GLU
1	D	329	ILE
1	D	333	ASP
1	D	334	LEU
1	D	337	GLU
1	D	341	ASP
1	D	349	ARG
1	D	352	TYR
1	D	367	ASP

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Mol	Chain	Res	Type
1	D	369	LEU
1	D	386	VAL
1	D	396	SER
1	D	404	GLU
1	D	428	ASP
1	D	432	LEU
1	D	434	ASN
1	D	435	VAL
1	D	443	LEU
1	D	457	ASN
1	D	460	ASN
1	D	469	GLN
1	D	478	VAL
1	D	491	SER
1	D	493	LEU
1	D	499	LYS
1	E	133	LEU
1	E	143	ARG
1	E	154	ILE
1	E	175	GLN
1	E	199	THR
1	E	203	LEU
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	260	VAL
1	E	271	GLU
1	E	289	LEU
1	E	308	LEU
1	E	320	LEU
1	E	329	ILE
1	E	333	ASP
1	E	334	LEU
1	E	335	GLN
1	E	337	GLU
1	E	341	ASP
1	E	347	MET
1	E	349	ARG
1	E	375	ARG

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Mol	Chain	Res	Type
1	E	383	LYS
1	E	386	VAL
1	E	396	SER
1	E	428	ASP
1	E	434	ASN
1	E	435	VAL
1	E	440	PHE
1	E	442	VAL
1	E	443	LEU
1	E	457	ASN
1	E	460	ASN
1	E	469	GLN
1	E	488	ASN
1	E	491	SER
1	E	493	LEU
1	E	499	LYS
1	F	67	THR
1	F	69	SER
1	F	73	GLN
1	F	77	ASN
1	F	78	ILE
1	F	79	SER
1	F	113	LEU
1	F	114	HIS
1	F	115	GLU
1	F	133	LEU
1	F	154	ILE
1	F	169	ARG
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	248	VAL
1	F	271	GLU
1	F	283	LYS
1	F	286	MET
1	F	303	LYS
1	F	329	ILE
1	F	330	ASN

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Mol	Chain	Res	Type
1	F	333	ASP
1	F	334	LEU
1	F	337	GLU
1	F	341	ASP
1	F	353	LYS
1	F	369	LEU
1	F	374	GLN
1	F	383	LYS
1	F	396	SER
1	F	404	GLU
1	F	428	ASP
1	F	432	LEU
1	F	434	ASN
1	F	435	VAL
1	F	440	PHE
1	F	443	LEU
1	F	457	ASN
1	F	460	ASN
1	F	469	GLN
1	F	488	ASN
1	F	491	SER
1	F	493	LEU
1	F	499	LYS
1	G	67	THR
1	G	69	SER
1	G	78	ILE
1	G	79	SER
1	G	80	THR
1	G	88	LEU
1	G	97	GLN
1	G	115	GLU
1	G	133	LEU
1	G	143	ARG
1	G	175	GLN
1	G	177	LEU
1	G	199	THR
1	G	206	ASP
1	G	209	LYS
1	G	215	LYS
1	G	220	GLU
1	G	239	GLU
1	G	248	VAL

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Mol	Chain	Res	Type
1	G	260	VAL
1	G	264	LEU
1	G	271	GLU
1	G	283	LYS
1	G	289	LEU
1	G	308	LEU
1	G	320	LEU
1	G	321	PRO
1	G	329	ILE
1	G	333	ASP
1	G	334	LEU
1	G	335	GLN
1	G	337	GLU
1	G	341	ASP
1	G	347	MET
1	G	349	ARG
1	G	375	ARG
1	G	393	LEU
1	G	396	SER
1	G	407	GLU
1	G	418	VAL
1	G	428	ASP
1	G	434	ASN
1	G	435	VAL
1	G	439	VAL
1	G	440	PHE
1	G	443	LEU
1	G	457	ASN
1	G	469	GLN
1	G	488	ASN
1	G	491	SER
1	G	493	LEU
1	G	499	LYS
1	H	86	GLN
1	H	92	THR
1	H	93	SER
1	H	94	VAL
1	H	97	GLN
1	H	113	LEU
1	H	114	HIS
1	H	116	LEU
1	H	133	LEU

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Mol	Chain	Res	Type
1	H	154	ILE
1	H	168	VAL
1	H	169	ARG
1	H	175	GLN
1	H	199	THR
1	H	203	LEU
1	H	206	ASP
1	H	215	LYS
1	H	220	GLU
1	H	222	ILE
1	H	271	GLU
1	H	286	MET
1	H	291	GLU
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	337	GLU
1	H	341	ASP
1	H	347	MET
1	H	370	ARG
1	H	383	LYS
1	H	386	VAL
1	H	393	LEU
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	491	SER
1	H	493	LEU
1	H	499	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82)

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	451	GLN
1	A	457	ASN
1	A	469	GLN
1	A	488	ASN
1	A	496	ASN
1	B	73	GLN
1	B	98	GLN
1	B	175	GLN
1	B	176	ASN
1	B	249	ASN
1	B	374	GLN
1	B	433	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	438	ASN
1	C	441	ASN
1	C	451	GLN
1	C	457	ASN
1	C	488	ASN
1	C	496	ASN
1	D	98	GLN
1	D	112	ASN
1	D	213	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

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Mol	Chain	Res	Type
1	D	488	ASN
1	E	112	ASN
1	E	332	GLN
1	E	374	GLN
1	E	438	ASN
1	E	451	GLN
1	E	457	ASN
1	E	488	ASN
1	F	77	ASN
1	F	86	GLN
1	F	98	GLN
1	F	112	ASN
1	F	125	HIS
1	F	175	GLN
1	F	249	ASN
1	F	335	GLN
1	F	374	GLN
1	F	433	ASN
1	F	457	ASN
1	F	460	ASN
1	F	469	GLN
1	F	488	ASN
1	G	76	ASN
1	G	374	GLN
1	G	457	ASN
1	G	488	ASN
1	G	496	ASN
1	H	86	GLN
1	H	97	GLN
1	H	112	ASN
1	H	175	GLN
1	H	176	ASN
1	H	213	ASN
1	H	335	GLN
1	H	374	GLN
1	H	395	ASN
1	H	438	ASN
1	H	451	GLN
1	H	488	ASN
1	H	496	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	H	1503	-	12,12,12	2.06	3 (25%)	15,15,15	1.53	3 (20%)
2	NLG	D	1503	-	12,12,12	2.28	2 (16%)	15,15,15	2.13	7 (46%)

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	H	1503	-	-	0/13/13/13	-
2	NLG	D	1503	-	-	6/13/13/13	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1503	NLG	C8-C7	-5.93	1.38	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1503	NLG	C8-C7	-4.74	1.40	1.50
2	H	1503	NLG	CA-C	3.23	1.60	1.52
2	D	1503	NLG	CG-CD	2.97	1.57	1.50
2	H	1503	NLG	CG-CD	2.65	1.56	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1503	NLG	CB-CA-N2	4.75	120.31	110.91
2	D	1503	NLG	C8-C7-N2	3.18	121.39	116.12
2	H	1503	NLG	C-CA-N2	3.15	117.89	110.57
2	H	1503	NLG	O7-C7-C8	-3.00	116.72	122.05
2	D	1503	NLG	CA-N2-C7	2.61	128.90	121.58
2	D	1503	NLG	O7-C7-C8	-2.44	117.71	122.05
2	D	1503	NLG	C-CA-N2	-2.28	105.28	110.57
2	D	1503	NLG	CG-CB-CA	-2.18	109.14	113.16
2	H	1503	NLG	C8-C7-N2	2.14	119.67	116.12
2	D	1503	NLG	CB-CA-C	-2.14	105.27	110.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1503	NLG	CB-CA-N2-C7
2	D	1503	NLG	C8-C7-N2-CA
2	D	1503	NLG	O7-C7-N2-CA
2	D	1503	NLG	OXT-C-CA-N2
2	D	1503	NLG	O-C-CA-N2
2	D	1503	NLG	OE2-CD-CG-CB

There are no ring outliers.

2 monomers are involved in 12 short contacts:

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	405/464 (87%)	-0.52	0	100	100	46, 81, 135, 187	0
1	B	436/464 (93%)	-0.53	0	100	100	37, 73, 149, 245	0
1	C	436/464 (93%)	-0.56	0	100	100	35, 73, 151, 219	0
1	D	405/464 (87%)	-0.56	0	100	100	45, 80, 142, 205	0
1	E	405/464 (87%)	-0.30	1 (0%)	91	85	55, 102, 230, 344	0
1	F	436/464 (93%)	-0.51	1 (0%)	91	85	45, 83, 151, 217	0
1	G	436/464 (93%)	-0.39	1 (0%)	91	85	53, 96, 184, 263	0
1	H	422/464 (90%)	-0.51	0	100	100	50, 86, 170, 237	0
All	All	3381/3712 (91%)	-0.48	3 (0%)	92	90	35, 84, 166, 344	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	415	ASP	2.7
1	E	147	GLN	2.2
1	G	85	GLU	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NLG	H	1503	13/13	0.93	0.08	64,81,101,106	0
2	NLG	D	1503	13/13	0.94	0.08	48,59,72,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.