Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 04:11 am GMT

PDB ID	:	2W6G
Title	:	Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration: Hydration State 3.
Authors	:	Sanchez-Weatherby, J.; Felisaz, F.; Gobbo, A.; Huet, J.; Ravelli, R.B.G.; Bowler, M.W.; Cipriani, F.
Deposited on	:	2008-12-18
Resolution	:	6.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

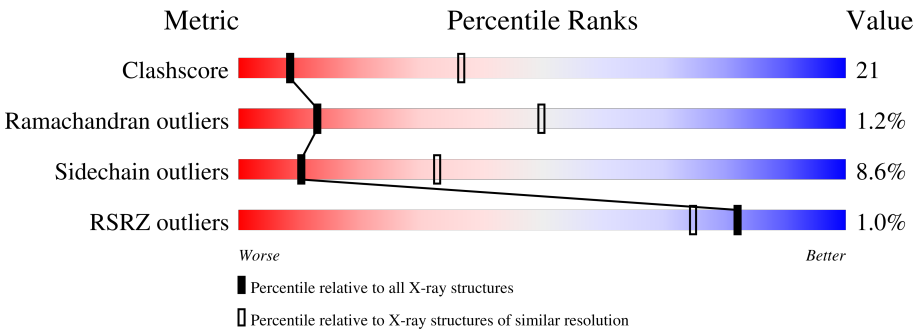
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 6.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1049 (8.00-3.90)
Ramachandran outliers	138981	1016 (8.00-3.86)
Sidechain outliers	138945	1017 (8.00-3.82)
RSRZ outliers	127900	1015 (8.20-3.78)

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 <=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	553	% 47% 33% 7% • 12%
1	B	553	47% 33% 6% • 13%
1	C	553	51% 33% • • 11%
2	D	528	% 55% 28% • • 12%
2	E	528	% 45% 36% 6% • 12%
2	F	528	% 57% 28% • 12%

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Mol	Chain	Length	Quality of chain
3	G	298	3% 34% 12% • 53%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22795 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 ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3715	2341	656	706	12	0	0	0
1	B	479	3656	2303	647	694	12	0	0	0
1	C	492	3748	2360	661	715	12	0	0	0

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	467	3539	2243	601	684	11	0	0	0
2	E	466	3530	2238	600	681	11	0	0	0
2	F	466	3530	2238	600	681	11	0	0	0

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

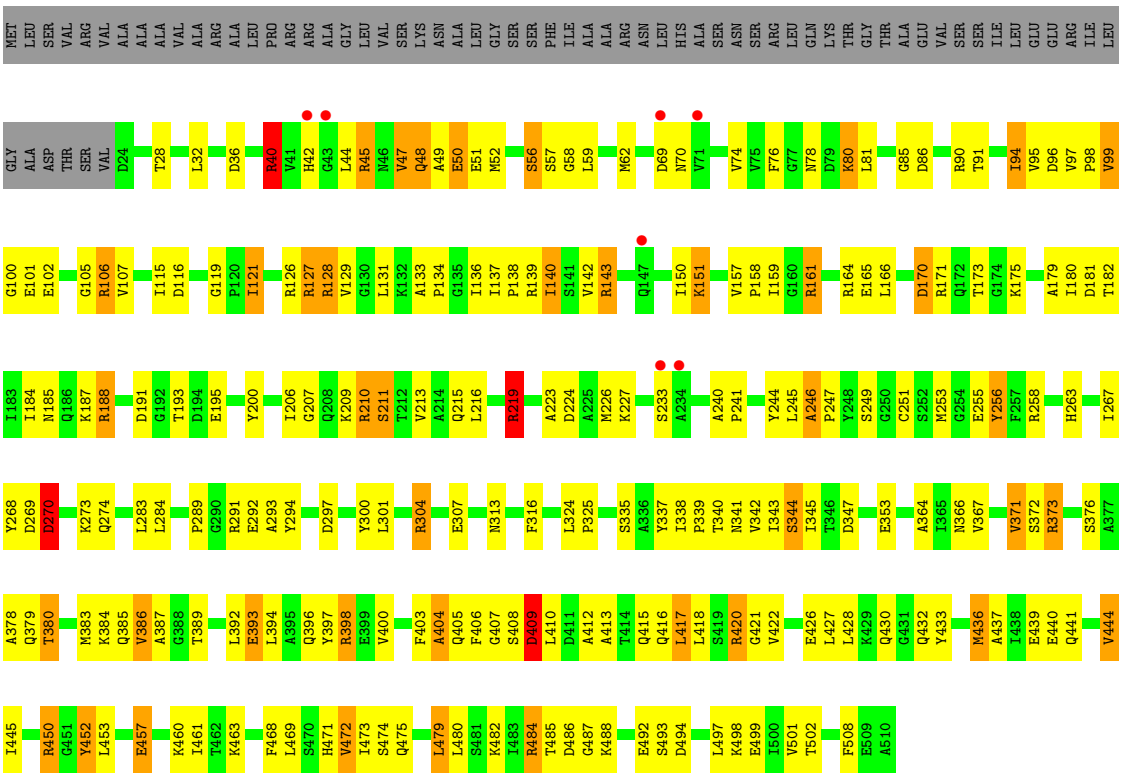
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	G	140	1077	671	195	205	6	0	0	0

3 Residue-property plots (i)

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.

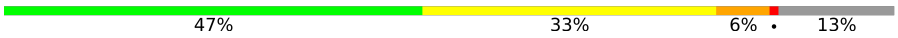
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

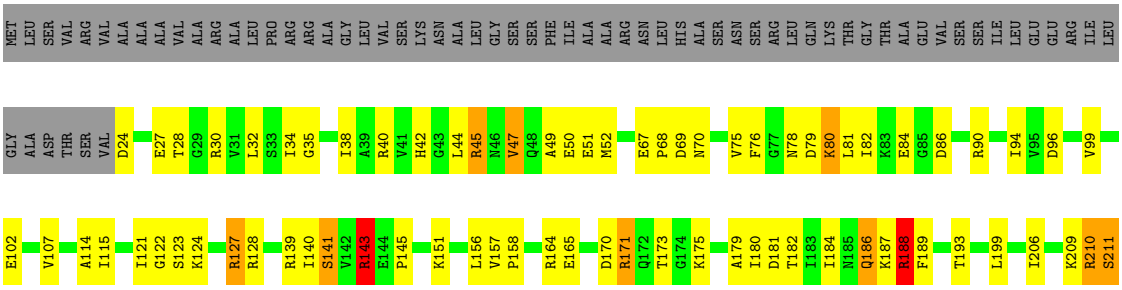
Chain A:

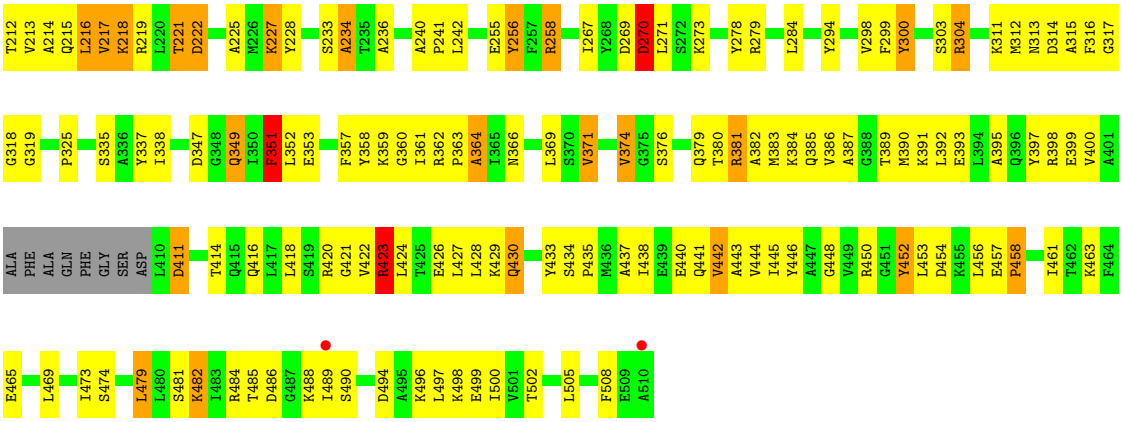


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

Chain B:

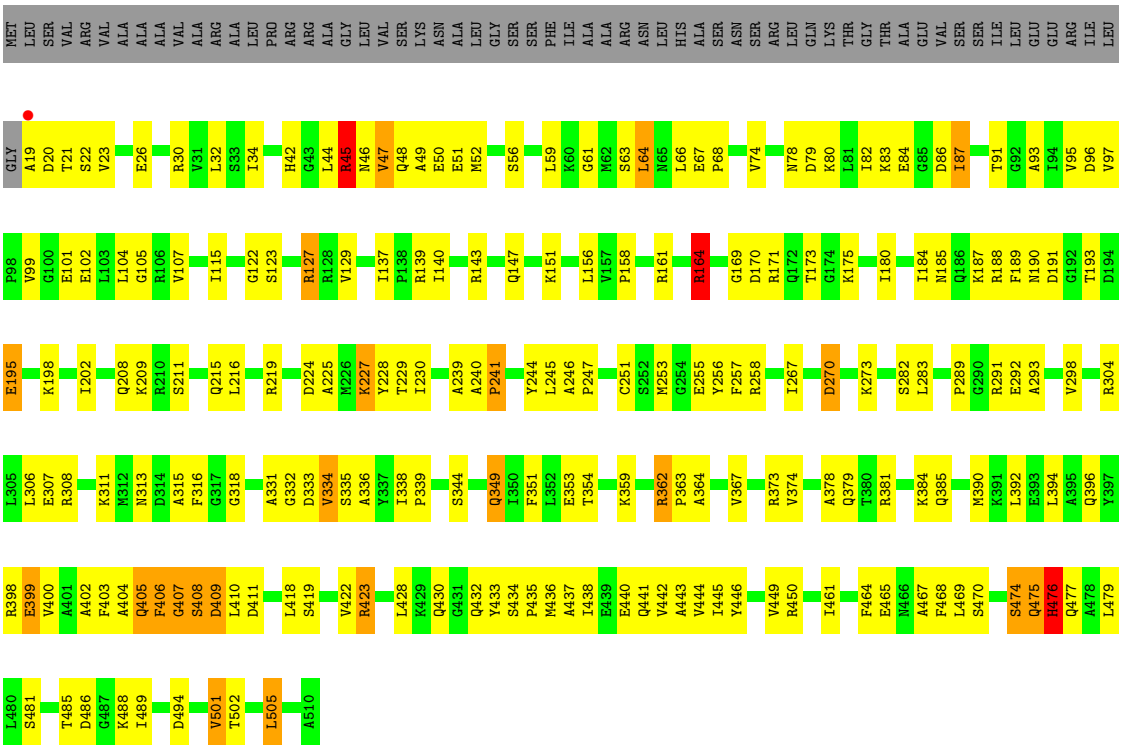






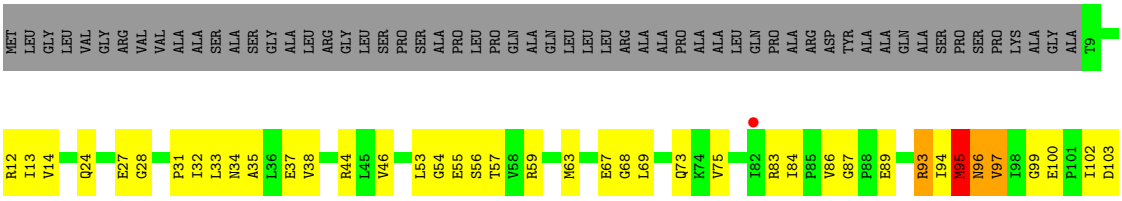
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

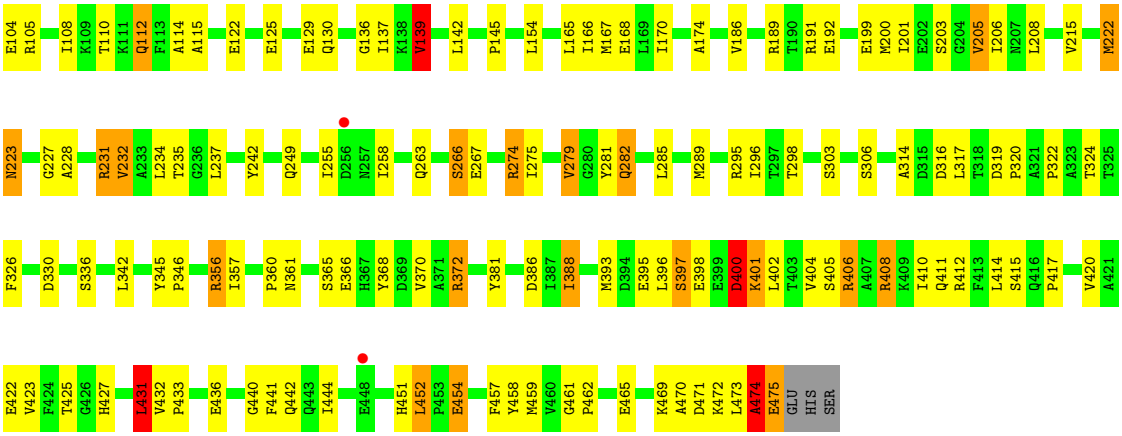
Chain C:



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

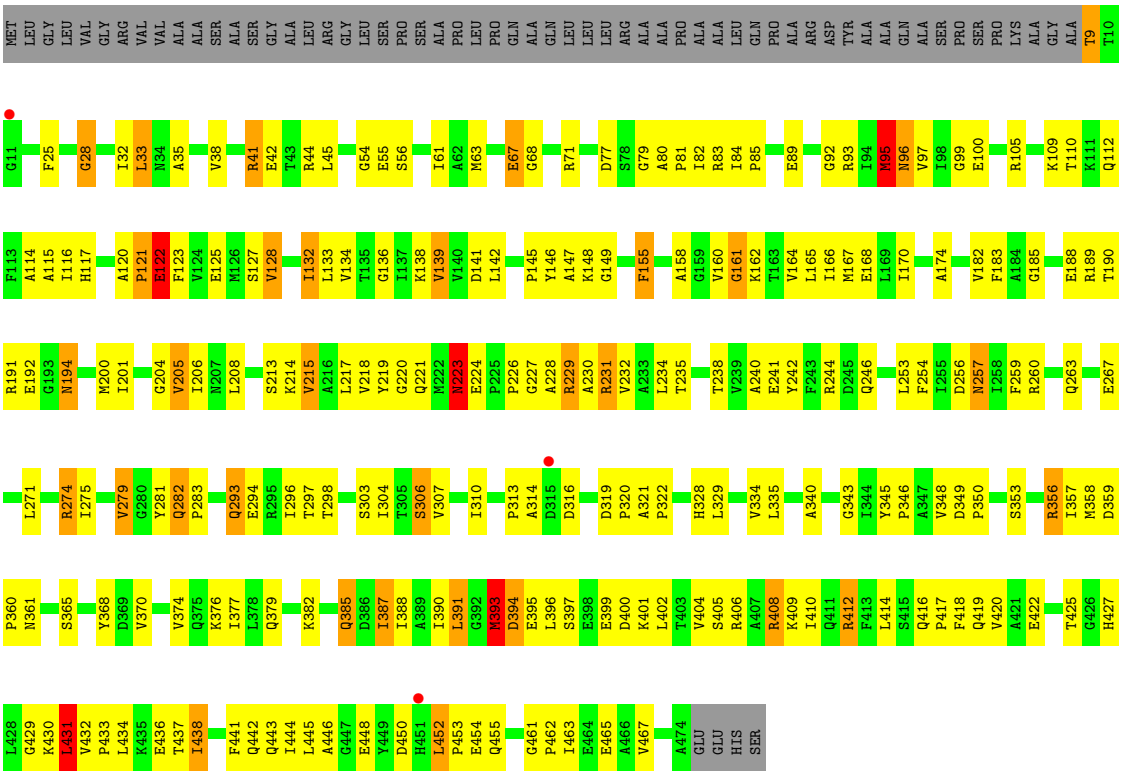
Chain D:





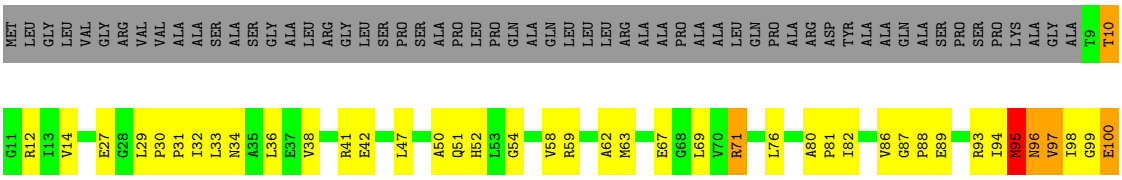
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

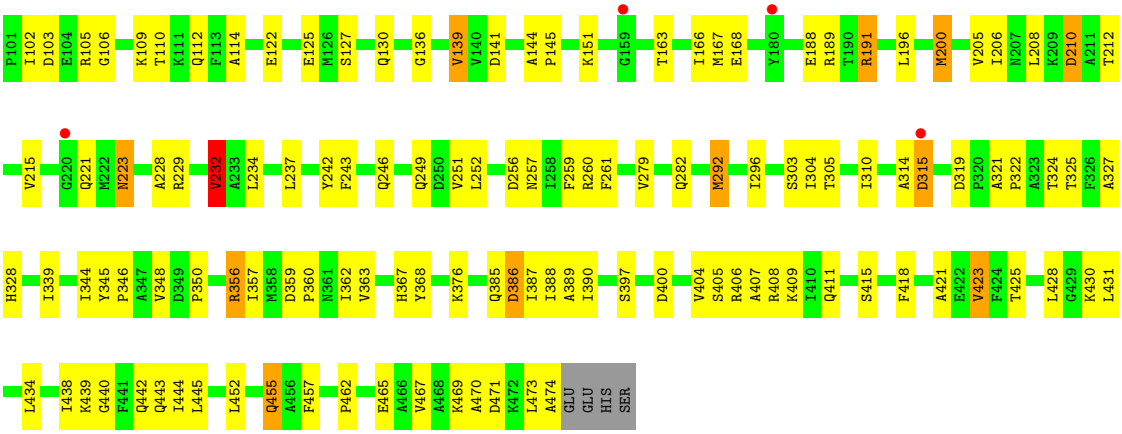
Chain E:



• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

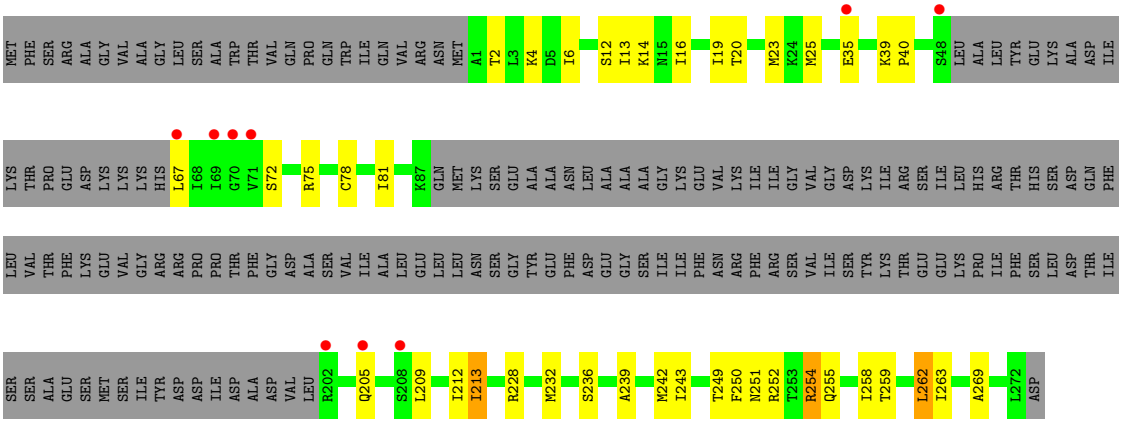
Chain F:





- Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	109.35Å 132.93Å 275.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.53 – 6.00 80.74 – 6.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (101.53-6.00) 65.8 (80.74-6.00)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 6.18Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.330 , (Not available) 0.329 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	156.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 37.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	22795	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.56% 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)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.60	0/3766	1.31	29/5080 (0.6%)
1	B	0.61	0/3704	1.36	34/4995 (0.7%)
1	C	0.62	0/3799	1.38	24/5126 (0.5%)
2	D	0.62	0/3596	1.36	23/4879 (0.5%)
2	E	0.60	0/3587	1.32	18/4867 (0.4%)
2	F	0.62	0/3587	1.36	27/4867 (0.6%)
3	G	0.33	0/1083	0.69	2/1448 (0.1%)
All	All	0.60	0/23122	1.33	157/31262 (0.5%)

There are no bond length outliers.

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	408	ARG	CD-NE-CZ	23.30	156.22	123.60
2	E	408	ARG	CD-NE-CZ	13.97	143.16	123.60
1	C	291	ARG	NE-CZ-NH2	-13.30	113.65	120.30
1	B	40	ARG	NE-CZ-NH1	13.08	126.84	120.30
1	B	279	ARG	NE-CZ-NH1	12.73	126.67	120.30
2	F	59	ARG	NE-CZ-NH1	-11.58	114.51	120.30
2	F	356	ARG	NE-CZ-NH1	11.56	126.08	120.30
2	D	406	ARG	NE-CZ-NH1	-11.39	114.61	120.30
2	D	408	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	B	219	ARG	NE-CZ-NH2	10.61	125.60	120.30
2	F	282	GLN	CB-CG-CD	10.30	138.39	111.60
1	C	164	ARG	NE-CZ-NH1	-9.90	115.35	120.30
1	B	40	ARG	CD-NE-CZ	9.89	137.44	123.60
1	C	258	ARG	NE-CZ-NH1	9.82	125.21	120.30
2	F	229	ARG	NE-CZ-NH1	-9.61	115.50	120.30
2	F	356	ARG	NE-CZ-NH2	-9.28	115.66	120.30
2	F	95	MET	CA-CB-CG	9.25	129.02	113.30
2	F	59	ARG	NE-CZ-NH2	9.21	124.90	120.30
2	D	44	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	C	161	ARG	NE-CZ-NH1	9.03	124.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	304	ARG	NE-CZ-NH1	-8.98	115.81	120.30
1	A	420	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	C	450	ARG	NE-CZ-NH2	-8.64	115.98	120.30
2	E	95	MET	CA-CB-CG	8.60	127.92	113.30
2	E	260	ARG	NE-CZ-NH1	-8.59	116.00	120.30
2	F	96	ASN	CB-CA-C	-8.59	93.22	110.40
1	A	398	ARG	NE-CZ-NH1	-8.37	116.11	120.30
2	E	83	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	A	373	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	A	450	ARG	NE-CZ-NH2	-8.15	116.22	120.30
2	F	229	ARG	NE-CZ-NH2	8.11	124.35	120.30
1	C	127	ARG	NE-CZ-NH1	-8.04	116.28	120.30
2	D	125	GLU	OE1-CD-OE2	-8.01	113.68	123.30
1	B	219	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	C	362	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	B	304	ARG	NE-CZ-NH2	7.84	124.22	120.30
2	E	229	ARG	NE-CZ-NH1	7.76	124.18	120.30
2	F	408	ARG	NE-CZ-NH2	7.65	124.12	120.30
1	C	450	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	279	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	B	270	ASP	CB-CA-C	-7.37	95.66	110.40
1	C	304	ARG	NE-CZ-NH2	7.33	123.96	120.30
2	D	93	ARG	NE-CZ-NH1	-7.22	116.69	120.30
1	A	270	ASP	CB-CA-C	-7.14	96.12	110.40
2	E	356	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	B	258	ARG	CD-NE-CZ	7.13	133.58	123.60
2	E	41	ARG	CD-NE-CZ	7.09	133.53	123.60
1	C	161	ARG	NE-CZ-NH2	-7.08	116.76	120.30
2	E	356	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	C	45	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	279	ARG	CD-NE-CZ	7.02	133.43	123.60
2	F	139	VAL	CB-CA-C	-7.00	98.11	111.40
1	A	450	ARG	NE-CZ-NH1	6.99	123.79	120.30
2	F	95	MET	C-N-CA	6.72	138.50	121.70
2	D	96	ASN	CB-CA-C	-6.70	97.00	110.40
1	B	349	GLN	CA-CB-CG	6.65	128.03	113.40
2	D	95	MET	C-N-CA	6.64	138.29	121.70
2	D	274	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	B	270	ASP	CB-CG-OD1	6.58	124.22	118.30
2	D	59	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	B	423	ARG	CD-NE-CZ	6.57	132.80	123.60
2	D	231	ARG	NE-CZ-NH1	6.54	123.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	256	ASP	CB-CG-OD1	6.53	124.18	118.30
2	E	44	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	C	308	ARG	NE-CZ-NH1	-6.45	117.07	120.30
1	A	106	ARG	CD-NE-CZ	6.45	132.63	123.60
1	A	398	ARG	NE-CZ-NH2	6.43	123.52	120.30
2	D	191	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	A	371	VAL	CB-CA-C	-6.42	99.20	111.40
1	A	372	SER	N-CA-CB	6.39	120.09	110.50
1	A	171	ARG	NE-CZ-NH2	6.37	123.49	120.30
1	A	170	ASP	CB-CG-OD1	6.37	124.03	118.30
2	F	189	ARG	NE-CZ-NH2	6.37	123.48	120.30
2	E	431	LEU	CA-CB-CG	6.36	129.93	115.30
1	A	127	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	D	372	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	C	308	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	B	300	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	C	291	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	C	381	ARG	CD-NE-CZ	6.20	132.28	123.60
1	A	210	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	E	274	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	127	ARG	CD-NE-CZ	6.17	132.23	123.60
1	C	476	HIS	N-CA-C	6.13	127.56	111.00
2	F	12	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	40	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	B	371	VAL	CB-CA-C	-6.08	99.85	111.40
2	F	97	VAL	CB-CA-C	-6.08	99.85	111.40
1	C	423	ARG	CD-NE-CZ	6.08	132.10	123.60
1	C	164	ARG	CD-NE-CZ	-6.05	115.13	123.60
2	D	222	MET	CB-CA-C	-5.94	98.52	110.40
1	A	269	ASP	C-N-CA	5.88	136.40	121.70
1	B	128	ARG	NE-CZ-NH1	5.84	123.22	120.30
3	G	254	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	210	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	297	ASP	CB-CG-OD1	5.73	123.45	118.30
2	F	191	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	D	139	VAL	CB-CA-C	-5.69	100.59	111.40
1	A	219	ARG	CD-NE-CZ	5.66	131.52	123.60
1	A	297	ASP	CB-CG-OD2	-5.66	113.21	118.30
2	F	103	ASP	CB-CG-OD2	-5.65	113.21	118.30
2	F	41	ARG	CG-CD-NE	5.64	123.64	111.80
2	D	474	ALA	C-N-CA	5.62	135.76	121.70
1	B	139	ARG	NE-CZ-NH1	5.62	123.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	398	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	B	337	TYR	CB-CG-CD1	5.58	124.35	121.00
1	A	304	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	A	233	SER	N-CA-CB	-5.57	102.14	110.50
2	D	454	GLU	CA-CB-CG	5.57	125.65	113.40
2	D	431	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	222	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	B	423	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	B	349	GLN	N-CA-CB	5.47	120.44	110.60
2	D	372	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	D	12	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	335	SER	CB-CA-C	-5.40	99.84	110.10
1	B	40	ARG	NE-CZ-NH2	-5.40	117.60	120.30
3	G	254	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	349	GLN	CB-CA-C	-5.35	99.70	110.40
1	C	170	ASP	CB-CG-OD1	5.32	123.08	118.30
2	F	191	ARG	CD-NE-CZ	5.31	131.04	123.60
1	B	45	ARG	CB-CG-CD	-5.31	97.80	111.60
1	C	241	PRO	N-CA-CB	5.30	109.66	103.30
1	C	171	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	188	ARG	CG-CD-NE	5.25	122.83	111.80
1	B	143	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	161	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	E	231	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	B	351	PHE	N-CA-CB	5.18	119.92	110.60
2	E	93	ARG	NE-CZ-NH1	-5.17	117.72	120.30
2	F	100	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	B	278	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	C	336	ALA	N-CA-CB	-5.15	102.89	110.10
1	A	258	ARG	CD-NE-CZ	5.15	130.81	123.60
2	D	316	ASP	CB-CG-OD2	-5.14	113.67	118.30
2	E	260	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	E	408	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	F	71	ARG	NE-CZ-NH2	5.13	122.86	120.30
1	A	270	ASP	CB-CG-OD1	5.13	122.91	118.30
2	F	232	VAL	CB-CA-C	-5.12	101.68	111.40
2	F	423	VAL	CB-CA-C	-5.11	101.69	111.40
2	D	356	ARG	CD-NE-CZ	-5.10	116.45	123.60
1	C	127	ARG	NH1-CZ-NH2	5.10	125.01	119.40
2	E	122	GLU	CA-CB-CG	5.09	124.61	113.40
2	E	96	ASN	N-CA-CB	-5.08	101.46	110.60
1	A	200	TYR	CA-CB-CG	-5.06	103.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	223	ASN	CB-CA-C	-5.06	100.28	110.40
2	F	303	SER	N-CA-CB	-5.05	102.92	110.50
2	D	400	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	300	TYR	CB-CG-CD1	5.04	124.02	121.00
1	A	40	ARG	CG-CD-NE	5.03	122.37	111.80
1	A	452	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	A	128	ARG	NE-CZ-NH1	-5.03	117.78	120.30
2	F	406	ARG	NE-CZ-NH1	-5.03	117.79	120.30
2	F	315	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	234	ALA	N-CA-C	-5.01	97.48	111.00
1	B	171	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3715	0	3813	184	0
1	B	3656	0	3764	156	58
1	C	3748	0	3843	163	56
2	D	3539	0	3593	158	0
2	E	3530	0	3587	217	0
2	F	3530	0	3587	124	2
3	G	1077	0	1139	66	0
All	All	22795	0	23326	961	58

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 21.

All (961) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:390:ILE:HD11	3:G:242:MET:CE	1.54	1.36
2:F:390:ILE:CD1	3:G:242:MET:CE	2.07	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:390:ILE:HG13	3:G:25:MET:SD	1.75	1.25
1:C:127:ARG:HH12	1:C:255:GLU:HB2	1.00	1.13
2:F:390:ILE:CD1	3:G:242:MET:HE3	1.77	1.09
2:F:390:ILE:HD11	3:G:242:MET:HE1	1.13	1.08
2:E:390:ILE:HG21	3:G:25:MET:HB3	1.30	1.06
1:C:215:GLN:HG3	2:F:356:ARG:HH22	0.95	1.05
1:A:291:ARG:CA	3:G:262:LEU:HD22	1.86	1.04
1:A:291:ARG:HA	3:G:262:LEU:HD22	1.04	1.01
1:A:291:ARG:HA	3:G:262:LEU:CD2	1.90	1.01
1:C:404:ALA:C	1:C:406:PHE:H	1.64	1.00
1:B:214:ALA:HA	2:E:123:PHE:CZ	1.96	0.99
1:C:215:GLN:HG3	2:F:356:ARG:NH2	1.77	0.98
2:E:223:ASN:HD22	2:E:223:ASN:H	1.00	0.98
2:E:314:ALA:CB	3:G:254:ARG:CZ	2.44	0.95
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.48	0.93
2:F:223:ASN:HD22	2:F:223:ASN:H	1.07	0.93
1:B:214:ALA:HB2	2:E:123:PHE:CE1	2.05	0.91
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.52	0.91
1:C:127:ARG:NH1	1:C:255:GLU:HB2	1.84	0.90
2:F:390:ILE:CD1	3:G:242:MET:HE1	1.81	0.90
1:A:215:GLN:HG3	2:D:356:ARG:NH1	1.88	0.88
2:D:395:GLU:OE2	3:G:75:ARG:NE	2.05	0.88
1:C:30:ARG:HE	1:C:87:ILE:HD11	1.37	0.88
2:E:89:GLU:HG2	2:E:110:THR:HG22	1.55	0.87
2:E:390:ILE:CG1	3:G:25:MET:SD	2.63	0.87
2:E:314:ALA:HB3	3:G:254:ARG:NH2	1.90	0.86
2:E:223:ASN:H	2:E:223:ASN:ND2	1.72	0.85
1:A:400:VAL:HG12	1:A:418:LEU:HD21	1.60	0.84
3:G:20:THR:HG22	3:G:236:SER:HB3	1.57	0.84
2:F:390:ILE:HD11	3:G:242:MET:SD	2.18	0.83
1:B:456:LEU:HD12	1:B:457:GLU:H	1.42	0.83
2:E:132:ILE:HD12	2:E:145:PRO:HB3	1.61	0.82
1:A:406:PHE:CD1	3:G:19:ILE:HD13	2.15	0.81
2:E:314:ALA:HB2	3:G:254:ARG:CZ	2.11	0.81
1:A:291:ARG:N	3:G:262:LEU:HD21	1.96	0.80
1:A:347:ASP:OD1	2:E:191:ARG:NH1	2.14	0.80
1:B:214:ALA:CA	2:E:123:PHE:CE1	2.65	0.79
1:B:141:SER:O	1:B:143:ARG:HD2	1.83	0.79
2:E:370:VAL:HG21	2:E:438:ILE:HG22	1.65	0.79
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.65	0.79
2:D:136:GLY:HA3	2:D:431:LEU:HD13	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:HG3	1:B:199:LEU:HB3	1.65	0.78
2:D:404:VAL:O	2:D:408:ARG:HG3	1.84	0.78
1:A:291:ARG:CA	3:G:262:LEU:CD2	2.55	0.77
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.50	0.76
2:F:390:ILE:HD13	3:G:242:MET:CE	2.14	0.76
1:B:379:GLN:HB3	1:B:384:LYS:HE2	1.68	0.76
2:D:282:GLN:H	2:D:282:GLN:HE21	1.30	0.76
2:F:390:ILE:HD13	3:G:242:MET:HE3	1.68	0.75
2:D:53:LEU:HD12	2:D:57:THR:HG22	1.66	0.75
2:F:130:GLN:HB3	2:F:357:ILE:HD11	1.67	0.75
2:D:433:PRO:HG2	2:D:436:GLU:HG2	1.70	0.74
2:E:89:GLU:HG3	2:E:109:LYS:O	1.87	0.74
2:F:223:ASN:H	2:F:223:ASN:ND2	1.85	0.74
1:B:214:ALA:CB	2:E:123:PHE:CE1	2.71	0.74
2:D:223:ASN:H	2:D:223:ASN:HD22	1.35	0.73
2:E:390:ILE:HG22	2:E:391:LEU:HD23	1.70	0.73
2:E:139:VAL:HG13	2:E:414:LEU:HD22	1.71	0.73
2:E:96:ASN:HB3	2:E:100:GLU:H	1.52	0.73
2:E:38:VAL:HG21	2:E:45:LEU:HD23	1.71	0.72
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.72	0.72
2:E:314:ALA:CB	3:G:254:ARG:NH2	2.50	0.72
2:E:183:PHE:HB3	2:E:217:LEU:HD22	1.72	0.72
1:B:209:LYS:HG2	2:E:294:GLU:OE2	1.89	0.71
2:F:89:GLU:HG3	2:F:109:LYS:O	1.89	0.71
2:D:275:ILE:HG23	3:G:269:ALA:HB2	1.73	0.71
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.71	0.71
2:D:96:ASN:HB2	2:D:100:GLU:H	1.56	0.71
2:D:393:MET:HE3	2:D:404:VAL:HG21	1.73	0.70
2:E:394:ASP:C	2:E:396:LEU:H	1.93	0.70
2:E:433:PRO:HD2	2:E:436:GLU:HB2	1.73	0.70
2:E:388:ILE:HG23	2:E:393:MET:HG3	1.73	0.70
2:E:345:TYR:HA	2:E:346:PRO:C	2.13	0.70
1:A:407:GLY:HA2	1:A:410:LEU:HD21	1.74	0.70
1:B:214:ALA:CA	2:E:123:PHE:CZ	2.74	0.69
1:A:215:GLN:HG3	2:D:356:ARG:HH12	1.57	0.69
1:C:211:SER:O	1:C:215:GLN:HG2	1.91	0.69
2:D:84:ILE:HB	2:D:95:MET:HE3	1.73	0.69
2:E:105:ARG:CZ	2:E:208:LEU:HD23	2.23	0.69
1:B:452:TYR:OH	1:B:498:LYS:HG3	1.92	0.69
1:A:97:VAL:HA	1:A:126:ARG:HH21	1.56	0.68
1:A:479:LEU:HA	1:A:482:LYS:HE3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:223:ASN:HD22	2:D:223:ASN:N	1.89	0.68
2:E:321:ALA:HB3	2:E:322:PRO:HD3	1.75	0.68
2:F:223:ASN:HD22	2:F:223:ASN:N	1.85	0.68
1:A:97:VAL:HB	1:A:98:PRO:HD2	1.76	0.68
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.68
1:C:385:GLN:OE1	1:C:488:LYS:HG2	1.93	0.68
1:A:134:PRO:O	1:A:139:ARG:NH2	2.27	0.67
1:A:440:GLU:O	1:A:444:VAL:HG13	1.94	0.67
1:B:156:LEU:HD22	1:B:391:LYS:HD2	1.77	0.67
2:E:223:ASN:HD22	2:E:223:ASN:N	1.84	0.67
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.75	0.67
2:F:252:LEU:HD23	2:F:305:THR:HB	1.75	0.67
2:E:313:PRO:HD2	2:E:322:PRO:HG3	1.75	0.67
2:F:390:ILE:HD12	3:G:242:MET:HE3	1.72	0.67
1:B:44:LEU:HB3	1:B:47:VAL:HG22	1.76	0.66
1:C:59:LEU:HD23	1:C:82:ILE:HD11	1.77	0.66
2:E:390:ILE:CG2	3:G:25:MET:HB3	2.18	0.66
3:G:14:LYS:HG3	3:G:243:ILE:HD12	1.76	0.66
1:C:344:SER:O	2:D:222:MET:CE	2.44	0.66
2:F:80:ALA:HB1	2:F:81:PRO:CD	2.25	0.66
2:F:409:LYS:HD3	2:F:457:PHE:CE2	2.30	0.66
1:C:418:LEU:O	1:C:422:VAL:HG23	1.94	0.66
2:E:359:ASP:OD2	2:E:361:ASN:HB2	1.96	0.66
2:D:223:ASN:H	2:D:223:ASN:ND2	1.93	0.65
1:C:173:THR:HG22	1:C:354:THR:HG22	1.77	0.65
2:D:167:MET:HB3	2:D:420:VAL:HG11	1.78	0.65
2:D:200:MET:HB3	2:D:206:ILE:HG13	1.79	0.65
2:F:314:ALA:O	2:F:315:ASP:HB2	1.95	0.65
1:C:44:LEU:O	1:C:47:VAL:HG22	1.96	0.65
1:B:188:ARG:HH21	1:B:437:ALA:HB2	1.62	0.65
1:C:99:VAL:HG22	1:C:253:MET:HA	1.78	0.65
2:E:314:ALA:HB1	3:G:254:ARG:NE	2.12	0.65
1:A:471:HIS:CE1	1:A:475:GLN:HG3	2.32	0.65
1:B:214:ALA:N	2:E:123:PHE:HE1	1.94	0.65
2:E:314:ALA:CB	3:G:254:ARG:NE	2.60	0.64
2:F:344:ILE:HG23	2:F:415:SER:HB3	1.78	0.64
2:F:136:GLY:HA3	2:F:431:LEU:CD1	2.26	0.64
1:C:188:ARG:HH21	1:C:437:ALA:HB2	1.62	0.64
1:C:488:LYS:HG2	1:C:489:ILE:H	1.63	0.64
2:D:54:GLY:O	2:D:55:GLU:HB2	1.96	0.64
2:E:136:GLY:HA3	2:E:431:LEU:HD13	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:SER:O	1:C:423:ARG:HG2	1.98	0.64
2:E:346:PRO:HG3	2:E:418:PHE:CZ	2.33	0.64
1:B:437:ALA:O	1:B:440:GLU:N	2.30	0.64
1:C:404:ALA:C	1:C:406:PHE:N	2.44	0.64
2:F:136:GLY:HA3	2:F:431:LEU:HD12	1.80	0.64
1:A:376:SER:HB3	1:A:384:LYS:HE2	1.78	0.64
1:B:214:ALA:HA	2:E:123:PHE:HZ	1.59	0.64
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.80	0.64
2:F:200:MET:HG3	2:F:205:VAL:HG23	1.80	0.64
1:A:291:ARG:HH21	3:G:258:ILE:CD1	2.10	0.63
1:B:214:ALA:HA	2:E:123:PHE:CE1	2.32	0.63
2:E:443:GLN:HG2	2:E:448:GLU:OE2	1.98	0.63
2:F:200:MET:HG3	2:F:205:VAL:CG2	2.27	0.63
2:E:139:VAL:CG1	2:E:414:LEU:HD22	2.28	0.63
2:E:400:ASP:O	2:E:404:VAL:HG23	1.98	0.63
3:G:39:LYS:HB3	3:G:40:PRO:HD3	1.80	0.63
1:A:344:SER:O	2:E:189:ARG:NH2	2.32	0.63
2:F:94:ILE:HG22	2:F:102:ILE:HD11	1.80	0.63
2:E:425:THR:O	2:E:427:HIS:ND1	2.21	0.63
1:A:291:ARG:N	3:G:262:LEU:CD2	2.59	0.63
2:E:298:THR:HG23	2:E:303:SER:HB3	1.81	0.63
2:F:363:VAL:HG23	2:F:367:HIS:HB3	1.81	0.63
2:E:204:GLY:O	2:E:206:ILE:N	2.32	0.62
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.64	0.62
1:A:376:SER:C	1:A:378:ALA:H	2.02	0.62
1:B:67:GLU:O	2:F:71:ARG:NH1	2.31	0.62
1:B:397:TYR:CD1	1:B:421:GLY:HA3	2.34	0.62
1:C:52:MET:O	1:C:91:THR:HB	1.99	0.62
2:E:138:LYS:HE2	2:E:432:VAL:HG21	1.81	0.62
1:C:151:LYS:HE3	1:C:430:GLN:HG3	1.82	0.62
1:A:341:ASN:O	1:A:345:ILE:HG13	1.99	0.62
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.34	0.62
1:A:394:LEU:HD11	1:A:428:LEU:HD11	1.82	0.62
1:B:389:THR:HA	1:B:392:LEU:CD1	2.29	0.62
1:A:209:LYS:NZ	2:D:330:ASP:OD1	2.31	0.61
2:E:422:GLU:HG2	2:E:427:HIS:O	1.99	0.61
1:B:102:GLU:HG3	1:B:122:GLY:O	2.00	0.61
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.82	0.61
2:D:396:LEU:HD22	2:D:400:ASP:CB	2.30	0.61
1:A:283:LEU:HD21	1:A:289:PRO:HB3	1.83	0.61
2:E:224:GLU:O	2:E:229:ARG:NH1	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:GLU:O	1:C:293:ALA:HB3	2.00	0.61
1:A:291:ARG:HH21	3:G:258:ILE:HD13	1.66	0.61
1:B:389:THR:HA	1:B:392:LEU:HD12	1.82	0.60
1:B:362:ARG:HA	1:B:363:PRO:C	2.22	0.60
1:C:373:ARG:CZ	2:D:189:ARG:NH2	2.64	0.60
2:E:201:ILE:HD13	2:E:208:LEU:HD11	1.82	0.60
1:B:184:ILE:HG22	1:B:435:PRO:HG2	1.81	0.60
1:A:52:MET:O	1:A:91:THR:HG23	2.02	0.60
1:B:422:VAL:O	1:B:426:GLU:HG2	2.00	0.60
1:A:166:LEU:HA	1:A:325:PRO:HD2	1.83	0.60
1:A:270:ASP:OD1	1:A:273:LYS:HG3	2.01	0.60
1:B:218:LYS:HG2	2:E:128:VAL:HG11	1.84	0.60
2:E:32:ILE:O	2:E:33:LEU:HB2	2.02	0.60
2:E:394:ASP:C	2:E:396:LEU:N	2.54	0.60
1:A:457:GLU:CB	1:A:460:LYS:HD3	2.31	0.60
1:B:51:GLU:HA	1:B:94:ILE:HA	1.83	0.60
2:D:89:GLU:HG2	2:D:110:THR:HG22	1.83	0.60
2:D:93:ARG:HG3	2:D:93:ARG:HH11	1.66	0.60
2:E:419:GLN:HG3	2:E:429:GLY:HA3	1.84	0.60
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.83	0.60
1:C:362:ARG:HA	1:C:363:PRO:C	2.21	0.60
1:A:121:ILE:HD13	1:A:121:ILE:H	1.66	0.60
2:E:397:SER:H	2:E:400:ASP:HB2	1.66	0.60
1:A:40:ARG:HH11	1:A:40:ARG:HG3	1.66	0.59
1:B:438:ILE:O	1:B:442:VAL:HG22	2.02	0.59
1:B:479:LEU:HD11	1:B:497:LEU:HD13	1.83	0.59
2:E:149:GLY:HA2	2:E:304:ILE:O	2.02	0.59
1:B:499:GLU:O	1:B:502:THR:HB	2.03	0.59
2:F:96:ASN:HD22	2:F:100:GLU:HB2	1.68	0.59
1:A:157:VAL:N	1:A:158:PRO:CD	2.65	0.59
1:B:214:ALA:N	2:E:123:PHE:CE1	2.70	0.59
1:C:102:GLU:OE2	1:C:123:SER:HA	2.03	0.59
2:D:263:GLN:O	2:D:267:GLU:HG3	2.03	0.59
1:B:400:VAL:HB	1:B:418:LEU:HD21	1.85	0.59
2:E:408:ARG:O	2:E:412:ARG:HG3	2.02	0.59
1:B:170:ASP:O	1:B:175:LYS:HE2	2.03	0.59
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.37	0.59
1:B:452:TYR:O	1:B:453:LEU:HD23	2.03	0.59
2:F:105:ARG:NH1	2:F:208:LEU:HD23	2.18	0.59
3:G:19:ILE:HG22	3:G:23:MET:HE2	1.85	0.59
1:A:432:GLN:HB3	1:A:433:TYR:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:LYS:O	1:B:395:ALA:N	2.36	0.59
1:C:140:ILE:HD11	1:C:143:ARG:NH2	2.18	0.59
2:D:317:LEU:HD22	2:D:326:PHE:HZ	1.67	0.59
1:B:434:SER:N	1:B:435:PRO:HD3	2.18	0.59
1:C:313:ASN:OD1	1:C:316:PHE:HD1	1.85	0.59
2:D:186:VAL:HG13	2:D:232:VAL:HG23	1.85	0.59
2:F:122:GLU:HB2	2:F:125:GLU:HG3	1.84	0.59
1:C:407:GLY:HA2	1:C:410:LEU:HD11	1.84	0.58
1:C:374:VAL:HG11	1:C:378:ALA:HB2	1.85	0.58
1:A:376:SER:C	1:A:378:ALA:N	2.55	0.58
1:C:464:PHE:CE1	1:C:505:LEU:HD23	2.39	0.58
1:C:344:SER:O	2:D:222:MET:HE2	2.04	0.58
2:E:122:GLU:N	2:E:125:GLU:OE2	2.37	0.58
2:E:200:MET:HB3	2:E:205:VAL:HG23	1.84	0.58
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.85	0.58
1:B:352:LEU:HA	1:B:364:ALA:O	2.04	0.58
2:E:95:MET:CG	2:E:99:GLY:HA2	2.34	0.58
2:E:226:PRO:HB3	2:E:267:GLU:HB2	1.84	0.58
1:B:411:ASP:HB3	1:B:414:THR:OG1	2.03	0.58
1:C:396:GLN:HG3	2:D:458:TYR:CE2	2.38	0.58
1:C:406:PHE:O	1:C:408:SER:N	2.36	0.58
2:E:397:SER:C	2:E:399:GLU:N	2.58	0.58
1:A:472:VAL:HG23	1:A:480:LEU:HD11	1.85	0.58
2:E:138:LYS:O	2:E:142:LEU:HB3	2.04	0.58
1:C:396:GLN:NE2	2:D:342:LEU:O	2.35	0.57
2:D:237:LEU:HD13	2:D:296:ILE:HG12	1.85	0.57
2:E:433:PRO:HG2	2:E:436:GLU:HG2	1.86	0.57
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.87	0.57
1:B:393:GLU:OE1	1:B:424:LEU:HD11	2.05	0.57
1:C:184:ILE:HG22	1:C:435:PRO:HG2	1.87	0.57
1:C:404:ALA:O	1:C:406:PHE:N	2.37	0.57
1:A:291:ARG:NH2	3:G:258:ILE:HD13	2.19	0.57
2:E:158:ALA:C	2:E:160:VAL:H	2.08	0.57
2:F:440:GLY:O	2:F:444:ILE:HG13	2.04	0.57
1:B:51:GLU:OE2	1:B:90:ARG:HB3	2.05	0.57
1:C:78:ASN:ND2	1:C:80:LYS:HD3	2.19	0.57
2:E:77:ASP:OD1	2:E:79:GLY:N	2.34	0.57
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.85	0.57
1:A:406:PHE:CG	3:G:19:ILE:HG21	2.40	0.57
1:C:107:VAL:HG12	1:C:115:ILE:HD11	1.86	0.57
2:E:105:ARG:NH2	2:E:208:LEU:HA	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:PHE:CE1	1:B:362:ARG:HD3	2.40	0.57
2:E:246:GLN:HA	2:E:246:GLN:NE2	2.19	0.57
2:F:14:VAL:O	2:F:71:ARG:HG2	2.05	0.57
1:A:219:ARG:HH11	1:A:219:ARG:HB2	1.69	0.56
2:D:282:GLN:H	2:D:282:GLN:NE2	2.01	0.56
1:A:107:VAL:HG12	1:A:115:ILE:HD11	1.87	0.56
2:E:155:PHE:CE1	2:E:310:ILE:HD12	2.40	0.56
1:A:185:ASN:O	1:A:188:ARG:HG3	2.05	0.56
1:B:214:ALA:HB2	2:E:123:PHE:CD1	2.41	0.56
1:C:156:LEU:HD13	1:C:367:VAL:HG22	1.86	0.56
2:F:32:ILE:O	2:F:33:LEU:HB2	2.05	0.56
3:G:209:LEU:O	3:G:213:ILE:HG22	2.05	0.56
1:A:450:ARG:NH2	1:A:494:ASP:OD2	2.38	0.56
2:E:267:GLU:O	2:E:271:LEU:HG	2.05	0.56
1:A:209:LYS:HE3	1:A:211:SER:HB2	1.88	0.56
1:B:423:ARG:HE	1:B:458:PRO:HG3	1.71	0.56
1:C:408:SER:O	1:C:409:ASP:C	2.44	0.56
2:D:471:ASP:O	2:D:474:ALA:N	2.39	0.56
2:F:98:ILE:HG13	2:F:100:GLU:HG3	1.88	0.56
1:B:351:PHE:CE1	1:B:369:LEU:HB3	2.41	0.56
1:C:173:THR:CG2	1:C:354:THR:HG22	2.35	0.56
1:B:80:LYS:HG3	1:B:81:LEU:HD23	1.88	0.56
1:B:347:ASP:HB3	1:B:374:VAL:HG22	1.88	0.56
2:D:366:GLU:HG3	2:D:442:GLN:HE22	1.71	0.56
2:E:174:ALA:CB	2:E:214:LYS:HD3	2.35	0.56
1:C:219:ARG:HD3	1:C:433:TYR:CE1	2.41	0.55
1:C:344:SER:O	2:D:222:MET:HE1	2.05	0.55
2:F:324:THR:O	2:F:324:THR:HG22	2.05	0.55
1:C:187:LYS:HE2	1:C:191:ASP:OD2	2.05	0.55
2:D:473:LEU:C	2:D:475:GLU:H	2.08	0.55
2:E:84:ILE:HB	2:E:95:MET:HE1	1.88	0.55
2:E:138:LYS:HG3	2:E:416:GLN:OE1	2.06	0.55
2:E:244:ARG:HG3	2:E:303:SER:N	2.22	0.55
2:E:92:GLY:N	2:E:215:VAL:O	2.29	0.55
1:A:99:VAL:CG2	1:A:253:MET:HA	2.36	0.55
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.89	0.55
2:D:255:ILE:HG21	2:D:258:ILE:HD13	1.87	0.55
2:E:396:LEU:HB3	2:E:401:LYS:HG2	1.88	0.55
2:F:63:MET:CE	2:F:97:VAL:HG11	2.37	0.55
1:C:433:TYR:C	1:C:435:PRO:HD3	2.26	0.55
1:A:457:GLU:HB3	1:A:460:LYS:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:LEU:HD21	1:A:493:SER:HB3	1.89	0.55
1:C:403:PHE:CD2	2:D:408:ARG:CZ	2.89	0.55
2:D:425:THR:HG21	2:D:459:MET:HE1	1.88	0.55
1:C:394:LEU:HD22	1:C:398:ARG:HH21	1.71	0.55
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.42	0.55
1:A:207:GLY:HA3	1:A:273:LYS:HD3	1.90	0.54
1:C:405:GLN:C	1:C:406:PHE:HD1	2.11	0.54
2:D:451:HIS:CD2	2:D:452:LEU:HD23	2.42	0.54
2:D:473:LEU:O	2:D:475:GLU:N	2.40	0.54
1:B:423:ARG:HE	1:B:458:PRO:HD3	1.72	0.54
1:B:114:ALA:HB2	1:B:121:ILE:HD11	1.89	0.54
1:B:441:GLN:O	1:B:445:ILE:HG12	2.08	0.54
1:C:399:GLU:HG2	2:D:342:LEU:HD22	1.90	0.54
2:E:201:ILE:CD1	2:E:208:LEU:HD11	2.37	0.54
2:E:397:SER:O	2:E:401:LYS:HG3	2.07	0.54
1:A:159:ILE:HD12	1:A:165:GLU:HG2	1.88	0.54
1:A:373:ARG:HG3	1:A:373:ARG:HH11	1.72	0.54
1:B:479:LEU:HA	1:B:482:LYS:HE3	1.89	0.54
1:C:442:VAL:CG1	1:C:489:ILE:HD11	2.37	0.54
1:B:446:TYR:CD2	1:B:497:LEU:HD23	2.43	0.54
1:C:52:MET:HG3	1:C:61:GLY:O	2.07	0.54
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.42	0.54
1:C:102:GLU:HG2	1:C:122:GLY:O	2.06	0.54
2:D:388:ILE:HD12	2:D:393:MET:SD	2.48	0.54
2:E:263:GLN:O	2:E:267:GLU:HG3	2.07	0.54
2:D:122:GLU:OE1	2:D:122:GLU:HA	2.07	0.54
2:F:10:THR:HG23	2:F:76:LEU:HD12	1.88	0.54
2:F:439:LYS:HE3	2:F:443:GLN:HE22	1.73	0.54
2:F:390:ILE:CD1	3:G:242:MET:SD	2.86	0.54
2:D:83:ARG:HA	2:D:114:ALA:O	2.07	0.54
1:A:170:ASP:O	1:A:175:LYS:HE2	2.08	0.54
1:A:463:LYS:HD3	1:A:508:PHE:HZ	1.73	0.54
1:A:468:PHE:CE1	1:A:501:VAL:HG12	2.43	0.54
1:B:270:ASP:OD1	1:B:273:LYS:HG3	2.08	0.54
1:B:358:TYR:C	1:B:360:GLY:H	2.11	0.54
1:A:161:ARG:HH11	1:A:263:HIS:CG	2.26	0.53
1:B:44:LEU:O	1:B:47:VAL:HG22	2.09	0.53
1:B:456:LEU:HD12	1:B:457:GLU:N	2.20	0.53
1:A:100:GLY:HA2	1:A:256:TYR:CE1	2.42	0.53
2:D:396:LEU:HD22	2:D:400:ASP:HB3	1.89	0.53
3:G:249:THR:HA	3:G:252:ARG:NH1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ALA:HB1	1:C:241:PRO:HD2	1.90	0.53
2:D:356:ARG:O	2:D:356:ARG:HG2	2.09	0.53
2:D:431:LEU:C	2:D:431:LEU:HD12	2.29	0.53
2:F:292:MET:CE	2:F:296:ILE:HD11	2.38	0.53
3:G:39:LYS:HB3	3:G:40:PRO:CD	2.38	0.53
1:A:150:ILE:HA	1:A:430:GLN:OE1	2.08	0.53
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.91	0.53
1:A:452:TYR:OH	1:A:498:LYS:HG3	2.08	0.53
2:D:417:PRO:HB3	2:D:459:MET:HE3	1.91	0.53
2:E:174:ALA:HB2	2:E:214:LYS:HD3	1.89	0.53
2:F:96:ASN:HB2	2:F:100:GLU:H	1.74	0.53
1:A:406:PHE:HB2	3:G:19:ILE:HG23	1.90	0.53
2:D:167:MET:CB	2:D:420:VAL:HG11	2.38	0.53
2:D:412:ARG:HH11	2:D:412:ARG:HG3	1.73	0.53
1:B:69:ASP:O	1:B:70:ASN:HB3	2.09	0.53
1:B:482:LYS:O	1:B:486:ASP:N	2.38	0.53
1:A:291:ARG:HG3	3:G:258:ILE:CG2	2.39	0.53
1:C:91:THR:HG22	1:C:93:ALA:H	1.72	0.53
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.24	0.53
2:D:136:GLY:CA	2:D:431:LEU:HD13	2.37	0.53
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.91	0.53
2:E:9:THR:HG21	2:E:28:GLY:O	2.09	0.52
2:E:218:VAL:HG11	2:E:235:THR:CG2	2.38	0.52
1:B:140:ILE:HG23	1:B:311:LYS:HG3	1.92	0.52
2:D:473:LEU:C	2:D:475:GLU:N	2.62	0.52
3:G:23:MET:SD	3:G:232:MET:HE2	2.50	0.52
1:B:180:ILE:O	1:B:181:ASP:C	2.47	0.52
1:B:180:ILE:CD1	1:B:216:LEU:HD21	2.39	0.52
1:B:423:ARG:HD2	1:B:461:ILE:HD11	1.92	0.52
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.92	0.52
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.75	0.52
2:D:412:ARG:HD2	2:D:454:GLU:HB3	1.90	0.52
2:E:80:ALA:HB1	2:E:81:PRO:HD2	1.91	0.52
2:E:82:ILE:HB	2:E:116:ILE:HD13	1.92	0.52
2:D:422:GLU:HG2	2:D:427:HIS:O	2.09	0.52
2:F:210:ASP:HB2	2:F:212:THR:HG23	1.91	0.52
1:C:64:LEU:HD23	1:C:74:VAL:HG21	1.92	0.52
1:C:443:ALA:O	1:C:446:TYR:HB3	2.10	0.52
2:D:366:GLU:CG	2:D:442:GLN:HE22	2.23	0.52
2:D:395:GLU:CD	3:G:75:ARG:HH21	2.13	0.52
2:E:97:VAL:HG13	2:E:232:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:VAL:HG22	1:B:442:VAL:HG12	1.91	0.52
1:C:140:ILE:HD11	1:C:143:ARG:HH22	1.74	0.52
1:C:267:ILE:N	1:C:267:ILE:HD12	2.25	0.52
1:C:270:ASP:OD1	1:C:273:LYS:HG3	2.09	0.52
2:D:96:ASN:CB	2:D:100:GLU:H	2.22	0.52
2:E:81:PRO:HG2	2:E:115:ALA:HB1	1.91	0.52
2:E:334:VAL:HG23	2:E:353:SER:HA	1.92	0.52
1:B:157:VAL:N	1:B:158:PRO:CD	2.73	0.52
2:E:25:PHE:O	2:E:56:SER:HB3	2.10	0.52
1:A:436:MET:HG3	1:A:441:GLN:HG2	1.91	0.52
1:A:457:GLU:HB2	1:A:460:LYS:HD3	1.92	0.52
1:C:190:ASN:HA	1:C:198:LYS:HG2	1.91	0.52
1:C:335:SER:O	2:D:314:ALA:HA	2.09	0.52
2:E:279:VAL:HG12	2:E:279:VAL:O	2.10	0.52
2:E:254:PHE:CD1	2:E:307:VAL:HB	2.45	0.51
1:C:45:ARG:NH2	1:C:68:PRO:O	2.44	0.51
1:C:156:LEU:HD11	1:C:428:LEU:HD13	1.91	0.51
2:E:377:ILE:HG21	2:E:410:ILE:CD1	2.40	0.51
1:A:187:LYS:HE2	1:A:191:ASP:OD2	2.11	0.51
1:B:489:ILE:HG22	1:B:494:ASP:HB2	1.93	0.51
2:D:381:TYR:HE2	2:D:411:GLN:HE22	1.56	0.51
1:A:140:ILE:HG21	1:A:313:ASN:HA	1.92	0.51
3:G:19:ILE:HG22	3:G:23:MET:CE	2.39	0.51
1:A:224:ASP:CG	1:A:227:LYS:HE3	2.31	0.51
2:E:444:ILE:HD11	2:E:463:ILE:HD11	1.93	0.51
1:C:436:MET:CE	1:C:469:LEU:HD21	2.41	0.51
2:E:293:GLN:HG3	2:E:328:HIS:CG	2.45	0.51
2:E:443:GLN:O	2:E:446:ALA:HB3	2.10	0.51
2:F:257:ASN:HB3	2:F:260:ARG:HG2	1.92	0.51
2:F:360:PRO:HD3	2:F:368:TYR:CD2	2.46	0.51
1:B:157:VAL:N	1:B:158:PRO:HD3	2.25	0.51
1:C:399:GLU:CG	2:D:342:LEU:HD22	2.41	0.51
2:E:377:ILE:HG21	2:E:410:ILE:HD12	1.92	0.51
1:A:209:LYS:HZ1	2:D:330:ASP:CG	2.13	0.51
1:C:23:VAL:HG12	1:C:23:VAL:O	2.11	0.51
2:D:275:ILE:HG23	3:G:269:ALA:CB	2.40	0.51
1:A:406:PHE:CB	3:G:19:ILE:HG23	2.41	0.50
2:E:218:VAL:HG11	2:E:235:THR:HG22	1.91	0.50
2:E:382:LYS:O	2:E:385:GLN:HB2	2.11	0.50
2:F:421:ALA:O	2:F:425:THR:HG23	2.11	0.50
1:A:140:ILE:HD11	1:A:143:ARG:NE	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ILE:HD11	1:C:79:ASP:CB	2.41	0.50
1:C:244:TYR:O	1:C:247:PRO:HD2	2.11	0.50
2:D:406:ARG:O	2:D:410:ILE:HG13	2.11	0.50
2:E:241:GLU:HA	2:E:304:ILE:HD11	1.94	0.50
2:E:275:ILE:O	2:E:283:PRO:HG3	2.12	0.50
1:B:151:LYS:NZ	1:B:429:LYS:O	2.45	0.50
2:F:386:ASP:O	2:F:389:ALA:HB3	2.12	0.50
1:A:45:ARG:HA	2:E:71:ARG:NH2	2.27	0.50
1:B:386:VAL:CG2	1:B:442:VAL:HG12	2.41	0.50
1:C:331:ALA:O	1:C:333:ASP:N	2.44	0.50
2:E:142:LEU:HD21	2:E:374:VAL:HG21	1.93	0.50
2:F:234:LEU:O	2:F:237:LEU:HB3	2.10	0.50
1:B:390:MET:CE	1:B:428:LEU:HD21	2.42	0.50
2:D:168:GLU:HG3	2:D:168:GLU:O	2.11	0.50
2:E:221:GLN:N	2:E:224:GLU:OE1	2.44	0.50
2:F:242:TYR:CD1	2:F:246:GLN:HG3	2.46	0.50
1:B:27:GLU:O	1:B:90:ARG:HG3	2.12	0.50
1:C:164:ARG:HD2	1:C:306:LEU:O	2.11	0.50
1:C:406:PHE:N	1:C:406:PHE:CD1	2.79	0.50
1:B:284:LEU:HD21	2:E:274:ARG:HD3	1.94	0.50
1:C:434:SER:N	1:C:435:PRO:HD3	2.27	0.50
1:C:359:LYS:O	2:F:376:LYS:HE2	2.11	0.50
2:E:155:PHE:HE1	2:E:310:ILE:HD12	1.77	0.50
2:F:86:VAL:HG11	2:F:114:ALA:HB3	1.93	0.50
1:C:96:ASP:O	1:C:97:VAL:HG13	2.12	0.49
1:C:225:ALA:HA	1:C:228:TYR:CE1	2.47	0.49
2:F:80:ALA:HB1	2:F:81:PRO:HD2	1.94	0.49
1:C:403:PHE:CZ	2:D:408:ARG:HD2	2.48	0.49
2:D:14:VAL:HG11	2:D:24:GLN:HB2	1.95	0.49
2:D:154:LEU:HD22	2:D:165:LEU:HD23	1.92	0.49
1:A:313:ASN:O	1:A:316:PHE:N	2.37	0.49
1:B:96:ASP:HB2	1:B:127:ARG:O	2.12	0.49
1:B:463:LYS:HE2	1:B:508:PHE:CZ	2.48	0.49
1:C:30:ARG:HA	1:C:86:ASP:O	2.12	0.49
2:D:96:ASN:HB2	2:D:100:GLU:N	2.27	0.49
2:F:96:ASN:ND2	2:F:100:GLU:HB2	2.26	0.49
1:A:137:ILE:N	1:A:138:PRO:CD	2.75	0.49
1:C:307:GLU:HG3	2:D:223:ASN:HB3	1.95	0.49
1:A:294:TYR:HB2	1:A:337:TYR:HE2	1.76	0.49
1:C:392:LEU:HD11	2:D:425:THR:HA	1.95	0.49
2:D:84:ILE:HD12	2:D:95:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:463:ILE:O	2:E:467:VAL:HG23	2.12	0.49
1:A:136:ILE:HG13	2:E:194:ASN:HB2	1.93	0.49
1:A:240:ALA:N	1:A:241:PRO:HD2	2.27	0.49
2:D:83:ARG:HA	2:D:115:ALA:HA	1.95	0.49
2:D:93:ARG:HG3	2:D:93:ARG:NH1	2.27	0.49
2:F:409:LYS:HD3	2:F:457:PHE:HE2	1.78	0.49
1:C:402:ALA:O	1:C:405:GLN:HG3	2.12	0.49
2:E:54:GLY:O	2:E:55:GLU:HB2	2.13	0.49
1:A:245:LEU:O	1:A:246:ALA:C	2.52	0.49
1:B:107:VAL:HG12	1:B:115:ILE:CG1	2.42	0.49
1:C:362:ARG:HG3	1:C:362:ARG:NH1	2.27	0.49
1:C:396:GLN:HG3	2:D:458:TYR:CZ	2.48	0.49
2:D:136:GLY:HA2	2:D:432:VAL:O	2.12	0.49
1:A:94:ILE:HG12	1:A:95:VAL:N	2.27	0.49
1:B:99:VAL:HG21	1:B:127:ARG:HB3	1.94	0.49
2:D:360:PRO:HD3	2:D:368:TYR:CE2	2.48	0.49
2:E:227:GLY:O	2:E:230:ALA:HB3	2.13	0.49
1:B:24:ASP:O	1:B:28:THR:HB	2.12	0.48
1:B:423:ARG:HE	1:B:458:PRO:CD	2.26	0.48
2:E:462:PRO:HD2	2:E:465:GLU:HG3	1.94	0.48
3:G:39:LYS:N	3:G:40:PRO:HD2	2.28	0.48
1:A:373:ARG:HG3	1:A:373:ARG:NH1	2.28	0.48
1:B:211:SER:O	1:B:215:GLN:HG3	2.13	0.48
1:B:311:LYS:HD2	1:B:312:MET:O	2.13	0.48
2:D:397:SER:O	2:D:400:ASP:N	2.45	0.48
2:F:163:THR:O	2:F:167:MET:HG2	2.12	0.48
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.78	0.48
2:F:321:ALA:HB3	2:F:322:PRO:HD3	1.95	0.48
2:F:339:ILE:HG22	2:F:344:ILE:HB	1.95	0.48
2:F:82:ILE:HD13	2:F:98:ILE:HG22	1.96	0.48
1:A:300:TYR:O	1:A:304:ARG:HG2	2.13	0.48
1:A:380:THR:O	1:A:384:LYS:HG3	2.12	0.48
1:A:444:VAL:CG1	1:A:469:LEU:HD13	2.44	0.48
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.95	0.48
2:E:134:VAL:HG13	2:E:141:ASP:OD2	2.13	0.48
2:F:168:GLU:OE1	2:F:418:PHE:HB3	2.12	0.48
1:B:351:PHE:HE1	1:B:369:LEU:O	1.96	0.48
1:C:52:MET:HE3	1:C:95:VAL:HG13	1.95	0.48
1:A:389:THR:O	1:A:393:GLU:HG2	2.13	0.48
1:B:49:ALA:O	1:B:50:GLU:HB2	2.13	0.48
1:B:218:LYS:HB2	2:E:128:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ILE:O	1:C:339:PRO:C	2.51	0.48
2:E:360:PRO:HD3	2:E:368:TYR:CD1	2.49	0.48
2:F:360:PRO:HD3	2:F:368:TYR:CE2	2.48	0.48
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.49	0.48
1:B:427:LEU:HD11	1:B:448:GLY:HA3	1.95	0.48
1:C:403:PHE:CD2	2:D:408:ARG:NH1	2.82	0.48
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.41	0.48
2:F:357:ILE:HD12	2:F:362:ILE:HG21	1.95	0.48
2:F:467:VAL:O	2:F:470:ALA:HB3	2.14	0.48
1:A:49:ALA:O	1:A:50:GLU:HB2	2.13	0.48
1:A:406:PHE:CB	3:G:19:ILE:CG2	2.92	0.48
1:A:485:THR:HG22	1:A:486:ASP:N	2.29	0.48
1:B:171:ARG:HG3	1:B:171:ARG:HH11	1.79	0.48
1:B:300:TYR:O	1:B:304:ARG:HG2	2.13	0.48
2:E:416:GLN:HG3	2:E:417:PRO:HD2	1.96	0.48
2:E:444:ILE:HD11	2:E:463:ILE:CD1	2.43	0.48
1:A:100:GLY:HA2	1:A:256:TYR:CD1	2.49	0.48
1:A:417:LEU:HD23	1:A:417:LEU:H	1.77	0.48
1:B:240:ALA:N	1:B:241:PRO:CD	2.77	0.48
1:C:313:ASN:OD1	1:C:315:ALA:HB3	2.14	0.48
2:E:253:LEU:O	2:E:306:SER:HA	2.14	0.48
2:F:88:PRO:HD2	2:F:89:GLU:OE2	2.14	0.47
1:B:383:MET:O	1:B:384:LYS:C	2.52	0.47
1:C:180:ILE:HG22	1:C:184:ILE:HD12	1.97	0.47
2:E:404:VAL:O	2:E:408:ARG:HG3	2.13	0.47
1:C:292:GLU:O	1:C:293:ALA:CB	2.63	0.47
2:E:116:ILE:HA	2:E:238:THR:OG1	2.15	0.47
1:A:453:LEU:HD13	1:A:461:ILE:HG23	1.96	0.47
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.48	0.47
1:C:445:ILE:HG22	1:C:449:VAL:CG2	2.44	0.47
2:D:32:ILE:O	2:D:33:LEU:HB2	2.14	0.47
2:E:374:VAL:O	2:E:377:ILE:HG22	2.14	0.47
2:F:36:LEU:N	2:F:36:LEU:HD23	2.29	0.47
1:A:166:LEU:HD13	1:A:342:VAL:HG12	1.95	0.47
1:A:376:SER:O	1:A:378:ALA:N	2.48	0.47
1:B:389:THR:HA	1:B:392:LEU:HG	1.97	0.47
2:E:61:ILE:HG13	2:E:61:ILE:O	2.14	0.47
2:F:96:ASN:HD22	2:F:100:GLU:CB	2.27	0.47
1:C:481:SER:O	1:C:485:THR:HB	2.14	0.47
2:E:259:PHE:CE2	2:E:263:GLN:HG2	2.50	0.47
1:A:240:ALA:HB3	1:A:241:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PHE:CE1	3:G:19:ILE:HD13	2.50	0.47
1:B:443:ALA:O	1:B:446:TYR:HB3	2.14	0.47
1:C:187:LYS:HE3	1:C:224:ASP:HB3	1.96	0.47
1:C:488:LYS:HG2	1:C:489:ILE:N	2.28	0.47
2:E:242:TYR:C	2:E:244:ARG:H	2.18	0.47
1:C:164:ARG:HD2	1:C:164:ARG:HH11	1.41	0.47
2:E:409:LYS:HZ2	2:E:450:ASP:HA	1.79	0.47
2:F:93:ARG:NH2	2:F:106:GLY:O	2.48	0.47
1:A:188:ARG:HE	1:A:437:ALA:HB2	1.80	0.47
1:A:209:LYS:HE3	1:A:211:SER:CB	2.45	0.47
1:B:400:VAL:HB	1:B:418:LEU:CD2	2.45	0.47
1:A:51:GLU:OE2	1:A:90:ARG:HB3	2.16	0.47
1:B:179:ALA:O	1:B:182:THR:HB	2.14	0.47
1:B:209:LYS:CG	2:E:294:GLU:OE2	2.59	0.47
1:B:481:SER:O	1:B:485:THR:HB	2.14	0.47
1:C:44:LEU:HB3	1:C:47:VAL:HG22	1.95	0.47
2:D:63:MET:HE3	2:D:228:ALA:HA	1.97	0.47
2:E:438:ILE:O	2:E:442:GLN:HB2	2.15	0.47
2:F:205:VAL:HG23	2:F:215:VAL:HG21	1.97	0.47
1:B:496:LYS:O	1:B:500:ILE:HG13	2.15	0.46
2:D:84:ILE:N	2:D:114:ALA:O	2.42	0.46
2:D:129:GLU:OE1	2:D:129:GLU:HA	2.14	0.46
2:D:154:LEU:HD13	2:D:165:LEU:HD23	1.96	0.46
2:D:469:LYS:O	2:D:473:LEU:HG	2.15	0.46
2:E:41:ARG:O	2:E:42:GLU:C	2.53	0.46
2:E:319:ASP:HA	3:G:255:GLN:OE1	2.15	0.46
2:E:431:LEU:HD12	2:E:431:LEU:O	2.15	0.46
1:A:313:ASN:OD1	1:A:316:PHE:HD2	1.98	0.46
1:C:156:LEU:HD11	1:C:428:LEU:CD1	2.46	0.46
1:A:85:GLY:O	1:A:86:ASP:C	2.53	0.46
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.46
1:C:91:THR:HG22	1:C:93:ALA:HB3	1.97	0.46
2:E:112:GLN:NE2	2:E:242:TYR:HE2	2.14	0.46
2:F:200:MET:CG	2:F:206:ILE:HG12	2.46	0.46
2:F:462:PRO:HG2	2:F:465:GLU:HG3	1.96	0.46
3:G:78:CYS:O	3:G:81:ILE:HD13	2.15	0.46
1:B:45:ARG:HH11	1:B:45:ARG:HD3	1.53	0.46
2:E:82:ILE:HB	2:E:116:ILE:CD1	2.45	0.46
2:E:204:GLY:C	2:E:206:ILE:N	2.68	0.46
2:F:346:PRO:HG3	2:F:418:PHE:HZ	1.80	0.46
1:A:127:ARG:HE	1:A:131:LEU:CD1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:89:GLU:HG2	2:F:110:THR:CG2	2.44	0.46
2:F:151:LYS:HD3	2:F:328:HIS:O	2.15	0.46
2:E:33:LEU:HD13	2:E:117:HIS:CG	2.50	0.46
2:F:339:ILE:CG2	2:F:344:ILE:HB	2.46	0.46
1:A:36:ASP:O	1:A:284:LEU:HD13	2.16	0.46
1:A:245:LEU:C	1:A:247:PRO:HD2	2.36	0.46
2:D:368:TYR:CE1	2:D:372:ARG:HG3	2.50	0.46
2:E:204:GLY:O	2:E:205:VAL:C	2.54	0.46
2:E:256:ASP:HA	2:E:257:ASN:HA	1.64	0.46
2:F:310:ILE:HD13	2:F:325:THR:HG21	1.98	0.46
2:E:343:GLY:O	2:E:345:TYR:HD1	1.99	0.46
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.15	0.46
1:C:392:LEU:CD1	2:D:425:THR:HA	2.45	0.46
2:E:120:ALA:HB1	2:E:121:PRO:HD2	1.98	0.46
2:E:223:ASN:ND2	2:E:223:ASN:N	2.46	0.46
1:C:441:GLN:O	1:C:445:ILE:HG12	2.15	0.46
2:D:130:GLN:HE22	2:D:356:ARG:HD3	1.81	0.46
2:D:289:MET:SD	2:D:324:THR:HG22	2.56	0.46
2:F:237:LEU:HD13	2:F:296:ILE:HG12	1.98	0.46
2:F:319:ASP:O	2:F:322:PRO:HD2	2.14	0.46
1:B:34:ILE:HD12	1:B:35:GLY:H	1.81	0.45
1:B:358:TYR:C	1:B:360:GLY:N	2.69	0.45
1:B:465:GLU:O	1:B:469:LEU:HB2	2.17	0.45
1:A:40:ARG:HH11	1:A:40:ARG:CG	2.27	0.45
1:A:300:TYR:HE1	2:E:223:ASN:O	1.99	0.45
1:A:339:PRO:O	1:A:343:ILE:HG13	2.16	0.45
1:B:269:ASP:HA	1:B:270:ASP:HA	1.77	0.45
1:C:251:CYS:O	1:C:255:GLU:HG3	2.16	0.45
2:F:96:ASN:HB2	2:F:100:GLU:N	2.31	0.45
1:A:412:ALA:HA	1:A:415:GLN:HB3	1.98	0.45
1:B:210:ARG:O	1:B:211:SER:C	2.54	0.45
1:C:102:GLU:HG2	1:C:122:GLY:C	2.36	0.45
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.34	0.45
1:C:432:GLN:O	1:C:433:TYR:HB2	2.16	0.45
2:E:146:TYR:O	2:E:357:ILE:HD11	2.16	0.45
2:E:443:GLN:HA	2:E:446:ALA:HB3	1.99	0.45
2:F:50:ALA:O	2:F:51:GLN:HB3	2.16	0.45
2:F:136:GLY:HA3	2:F:431:LEU:HD11	1.99	0.45
1:B:141:SER:HB2	1:B:143:ARG:NH1	2.31	0.45
1:B:271:LEU:HD12	1:B:325:PRO:HB2	1.98	0.45
2:D:432:VAL:HG13	2:D:433:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:405:SER:OG	2:E:406:ARG:N	2.49	0.45
2:F:469:LYS:O	2:F:473:LEU:HG	2.16	0.45
1:A:166:LEU:HD13	1:A:342:VAL:CG1	2.47	0.45
1:C:26:GLU:HB3	1:C:46:ASN:ND2	2.32	0.45
1:C:83:LYS:HB3	2:F:52:HIS:CE1	2.52	0.45
2:D:201:ILE:HD13	2:D:208:LEU:HD11	1.98	0.45
2:E:63:MET:CE	2:E:228:ALA:HA	2.46	0.45
2:E:388:ILE:HG23	2:E:393:MET:CG	2.43	0.45
1:A:151:LYS:HE2	1:A:427:LEU:O	2.17	0.45
1:A:398:ARG:HH11	1:A:398:ARG:HD2	1.53	0.45
2:D:440:GLY:O	2:D:444:ILE:HG13	2.16	0.45
2:E:281:TYR:CZ	2:E:321:ALA:HB2	2.52	0.45
2:F:455:GLN:H	2:F:455:GLN:CD	2.18	0.45
1:B:353:GLU:HG3	1:B:366:ASN:HB2	1.98	0.45
2:D:366:GLU:O	2:D:370:VAL:HG23	2.17	0.45
2:D:386:ASP:HB3	3:G:12:SER:CB	2.46	0.45
2:E:85:PRO:HD2	2:E:95:MET:CE	2.47	0.45
2:F:252:LEU:HD23	2:F:252:LEU:HA	1.81	0.45
1:A:179:ALA:O	1:A:182:THR:HB	2.17	0.45
1:B:27:GLU:OE1	1:B:90:ARG:HD3	2.16	0.45
1:C:84:GLU:OE1	2:F:54:GLY:HA2	2.17	0.45
1:C:158:PRO:HB3	1:C:379:GLN:HG3	1.99	0.45
1:C:476:HIS:ND1	1:C:476:HIS:N	2.64	0.45
2:D:237:LEU:HD21	2:D:295:ARG:HB2	1.97	0.45
2:D:452:LEU:HD12	2:D:457:PHE:CZ	2.52	0.45
2:E:147:ALA:HB2	2:E:357:ILE:HD13	1.99	0.45
1:A:142:VAL:HG22	1:A:161:ARG:O	2.16	0.45
1:A:213:VAL:O	1:A:216:LEU:HB3	2.16	0.45
1:A:283:LEU:HD11	1:A:293:ALA:HB1	1.99	0.45
1:C:67:GLU:HB3	1:C:68:PRO:HD2	1.98	0.45
1:C:390:MET:HE2	1:C:428:LEU:HD11	1.99	0.45
2:F:346:PRO:HG3	2:F:418:PHE:CZ	2.52	0.45
3:G:13:ILE:HD13	3:G:242:MET:SD	2.57	0.45
1:A:59:LEU:HD11	1:A:81:LEU:HD12	1.99	0.45
1:A:471:HIS:ND1	1:A:475:GLN:HG3	2.32	0.45
1:B:140:ILE:HG13	1:B:143:ARG:NH1	2.32	0.45
1:B:469:LEU:HG	1:B:473:ILE:HD11	1.98	0.45
1:C:311:LYS:HE3	1:C:318:GLY:O	2.17	0.45
2:E:461:GLY:HA3	2:E:462:PRO:HD3	1.73	0.45
2:F:243:PHE:O	2:F:249:GLN:HB2	2.16	0.45
1:B:76:PHE:HB3	1:B:242:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:103:ASP:O	2:D:104:GLU:HB2	2.17	0.44
2:D:231:ARG:O	2:D:234:LEU:N	2.50	0.44
2:D:345:TYR:HA	2:D:346:PRO:C	2.37	0.44
2:F:348:VAL:O	2:F:350:PRO:HD3	2.17	0.44
1:A:97:VAL:HG11	1:A:249:SER:HB2	1.99	0.44
1:A:244:TYR:HE1	1:A:301:LEU:HD11	1.83	0.44
1:B:300:TYR:HA	1:B:303:SER:OG	2.17	0.44
1:B:400:VAL:CG1	1:B:418:LEU:HD11	2.47	0.44
2:E:402:LEU:O	2:E:406:ARG:HG3	2.17	0.44
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.30	0.44
2:F:221:GLN:HA	2:F:221:GLN:NE2	2.31	0.44
2:F:345:TYR:HA	2:F:346:PRO:C	2.36	0.44
1:A:62:MET:HE2	1:A:76:PHE:HZ	1.82	0.44
1:A:379:GLN:HB2	1:A:384:LYS:HE3	2.00	0.44
1:B:32:LEU:HD21	1:B:42:HIS:HB2	1.99	0.44
1:C:403:PHE:CG	2:D:408:ARG:NH2	2.85	0.44
1:C:436:MET:HE1	1:C:469:LEU:HD21	2.00	0.44
2:D:95:MET:HG2	2:D:99:GLY:HA2	1.99	0.44
2:D:170:ILE:O	2:D:174:ALA:HB3	2.17	0.44
2:F:29:LEU:HD11	2:F:58:VAL:HG13	1.98	0.44
3:G:259:THR:O	3:G:263:ILE:HG12	2.17	0.44
1:A:385:GLN:OE1	1:A:488:LYS:HB2	2.17	0.44
1:B:80:LYS:HA	2:E:32:ILE:HB	1.98	0.44
1:B:423:ARG:HE	1:B:458:PRO:CG	2.30	0.44
1:C:52:MET:HE3	1:C:95:VAL:HG22	2.00	0.44
2:D:35:ALA:HB1	2:D:46:VAL:CG1	2.47	0.44
2:D:63:MET:HE1	2:D:227:GLY:O	2.17	0.44
2:E:114:ALA:HB3	2:E:238:THR:CG2	2.47	0.44
2:F:105:ARG:CZ	2:F:208:LEU:HD23	2.46	0.44
3:G:228:ARG:O	3:G:232:MET:HG2	2.17	0.44
1:B:437:ALA:O	1:B:438:ILE:C	2.54	0.44
1:C:219:ARG:HD3	1:C:433:TYR:HE1	1.81	0.44
1:C:474:SER:OG	1:C:475:GLN:N	2.49	0.44
2:D:298:THR:HG23	2:D:303:SER:HA	1.98	0.44
2:E:321:ALA:N	2:E:322:PRO:HD2	2.32	0.44
2:F:359:ASP:OD1	2:F:360:PRO:HD2	2.17	0.44
1:A:74:VAL:HG13	1:A:241:PRO:HG3	1.99	0.44
1:C:45:ARG:HH11	1:C:45:ARG:HD2	1.67	0.44
2:D:400:ASP:O	2:D:404:VAL:HG23	2.18	0.44
2:F:188:GLU:H	2:F:221:GLN:NE2	2.15	0.44
1:A:413:ALA:O	1:A:416:GLN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:THR:O	1:B:216:LEU:HB2	2.17	0.44
1:C:209:LYS:HE3	1:C:211:SER:OG	2.18	0.44
2:D:274:ARG:HH11	2:D:274:ARG:HD2	1.50	0.44
1:B:381:ARG:HG2	1:B:488:LYS:HG3	1.98	0.44
1:B:400:VAL:HG12	1:B:418:LEU:HD11	2.00	0.44
1:C:169:GLY:O	1:C:175:LYS:HE2	2.18	0.44
2:D:93:ARG:NH1	2:D:108:ILE:HG12	2.33	0.44
2:E:393:MET:HE3	2:E:396:LEU:HD12	1.99	0.44
1:A:97:VAL:N	1:A:127:ARG:O	2.41	0.44
1:A:251:CYS:O	1:A:255:GLU:HG3	2.18	0.44
1:A:392:LEU:O	1:A:396:GLN:HG3	2.18	0.44
1:B:107:VAL:HG12	1:B:115:ILE:HD11	2.00	0.44
1:C:59:LEU:HD23	1:C:82:ILE:CD1	2.45	0.44
2:F:407:ALA:O	2:F:411:GLN:HB2	2.18	0.44
1:A:460:LYS:N	1:A:460:LYS:HD2	2.32	0.43
1:C:489:ILE:HG22	1:C:494:ASP:HB2	1.99	0.43
2:D:412:ARG:O	2:D:415:SER:OG	2.33	0.43
2:E:397:SER:C	2:E:399:GLU:H	2.20	0.43
2:E:425:THR:C	2:E:427:HIS:N	2.72	0.43
3:G:6:ILE:HG21	3:G:250:PHE:HB2	2.00	0.43
1:A:140:ILE:CG2	1:A:313:ASN:HA	2.47	0.43
1:A:291:ARG:HH21	3:G:258:ILE:HD11	1.80	0.43
2:D:319:ASP:O	2:D:320:PRO:C	2.55	0.43
1:A:133:ALA:HB1	1:A:134:PRO:HD2	1.99	0.43
2:D:38:VAL:HG11	2:D:69:LEU:CD2	2.48	0.43
2:D:200:MET:HE3	2:D:215:VAL:HG21	2.00	0.43
2:D:461:GLY:HA3	2:D:462:PRO:HD3	1.74	0.43
2:E:136:GLY:HA2	2:E:432:VAL:O	2.18	0.43
1:A:52:MET:CG	1:A:95:VAL:HG22	2.48	0.43
1:B:294:TYR:CE2	1:B:338:ILE:HD13	2.53	0.43
1:C:137:ILE:HD13	1:C:137:ILE:HA	1.88	0.43
1:C:353:GLU:O	1:C:364:ALA:HB1	2.18	0.43
2:D:189:ARG:O	2:D:192:GLU:HB2	2.19	0.43
1:B:213:VAL:O	1:B:217:VAL:HG13	2.18	0.43
1:B:389:THR:HG22	1:B:392:LEU:HD12	2.00	0.43
1:C:32:LEU:HD21	1:C:42:HIS:HB2	2.01	0.43
1:C:404:ALA:HB1	1:C:410:LEU:HD11	1.99	0.43
2:D:108:ILE:HG22	2:D:110:THR:HG23	2.00	0.43
2:D:470:ALA:O	2:D:474:ALA:N	2.51	0.43
2:F:385:GLN:HA	2:F:388:ILE:HG12	2.01	0.43
2:F:439:LYS:HG2	2:F:443:GLN:NE2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.43
1:C:193:THR:O	1:C:195:GLU:OE1	2.36	0.43
2:E:376:LYS:O	2:E:379:GLN:HB2	2.18	0.43
2:F:141:ASP:HB3	2:F:434:LEU:HD13	2.01	0.43
2:F:257:ASN:OD1	2:F:259:PHE:HB3	2.17	0.43
1:B:151:LYS:NZ	1:B:427:LEU:O	2.47	0.43
1:B:450:ARG:HD3	1:B:450:ARG:HA	1.87	0.43
1:A:136:ILE:O	2:E:194:ASN:OD1	2.35	0.43
1:B:381:ARG:HA	1:B:384:LYS:HB2	2.01	0.43
1:B:434:SER:N	1:B:435:PRO:CD	2.81	0.43
1:C:245:LEU:O	1:C:246:ALA:C	2.56	0.43
2:E:310:ILE:HD11	2:E:329:LEU:HD11	2.00	0.43
2:F:95:MET:HG3	2:F:99:GLY:HA2	2.01	0.43
2:F:452:LEU:HD22	2:F:470:ALA:CB	2.49	0.43
1:A:62:MET:HE2	1:A:76:PHE:CZ	2.53	0.43
1:A:209:LYS:NZ	2:D:330:ASP:CG	2.70	0.43
1:B:385:GLN:NE2	1:B:489:ILE:HB	2.34	0.43
1:C:139:ARG:HB3	1:C:311:LYS:O	2.19	0.43
2:D:462:PRO:HD2	2:D:465:GLU:HG3	2.00	0.43
2:E:35:ALA:HB2	2:E:82:ILE:HG13	1.99	0.43
2:E:182:VAL:HG21	2:E:240:ALA:HB2	2.01	0.43
2:F:31:PRO:O	2:F:34:ASN:HB2	2.18	0.43
1:A:180:ILE:O	1:A:181:ASP:C	2.57	0.43
1:B:255:GLU:HG2	1:B:258:ARG:CZ	2.49	0.43
2:E:161:GLY:O	2:E:162:LYS:C	2.57	0.43
2:E:433:PRO:HG2	2:E:436:GLU:CG	2.48	0.43
1:C:185:ASN:HB2	1:C:435:PRO:HB3	2.00	0.42
2:D:386:ASP:CB	3:G:12:SER:HB3	2.49	0.42
2:D:412:ARG:HG3	2:D:412:ARG:NH1	2.33	0.42
2:E:296:ILE:HD13	2:E:306:SER:HB2	2.02	0.42
2:E:441:PHE:O	2:E:445:LEU:HG	2.19	0.42
2:F:144:ALA:N	2:F:145:PRO:CD	2.82	0.42
1:A:463:LYS:HD3	1:A:508:PHE:CZ	2.53	0.42
2:E:349:ASP:HA	2:E:350:PRO:HD2	1.87	0.42
3:G:239:ALA:O	3:G:243:ILE:HG12	2.18	0.42
1:A:45:ARG:HA	2:E:71:ARG:HH21	1.84	0.42
1:A:485:THR:C	1:A:487:GLY:N	2.73	0.42
1:C:49:ALA:O	1:C:50:GLU:HB2	2.19	0.42
1:C:51:GLU:HG2	1:C:52:MET:N	2.33	0.42
1:C:442:VAL:HG11	1:C:489:ILE:HD11	2.01	0.42
2:D:410:ILE:HG23	2:D:441:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:CG1	2:E:194:ASN:HB2	2.49	0.42
1:A:184:ILE:HD12	1:A:223:ALA:CB	2.50	0.42
1:A:291:ARG:HG3	3:G:258:ILE:HG23	2.00	0.42
1:A:340:THR:O	1:A:344:SER:HB3	2.19	0.42
1:B:389:THR:HA	1:B:392:LEU:CG	2.49	0.42
1:C:107:VAL:O	1:C:115:ILE:HG12	2.18	0.42
2:D:38:VAL:HG22	2:D:75:VAL:HG22	2.02	0.42
2:D:145:PRO:HB2	2:D:357:ILE:HD11	2.01	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB2	2.01	0.42
2:E:105:ARG:NE	2:E:208:LEU:HD23	2.33	0.42
2:F:122:GLU:OE1	2:F:122:GLU:HA	2.19	0.42
2:F:196:LEU:O	2:F:200:MET:HB2	2.19	0.42
1:A:96:ASP:HA	1:A:128:ARG:HA	2.02	0.42
1:A:136:ILE:HG21	1:A:136:ILE:HD13	1.83	0.42
1:A:485:THR:C	1:A:487:GLY:H	2.23	0.42
1:C:44:LEU:HD23	1:C:44:LEU:HA	1.92	0.42
1:C:49:ALA:N	1:C:66:LEU:HD11	2.34	0.42
1:C:224:ASP:OD1	1:C:227:LYS:HE3	2.20	0.42
1:C:423:ARG:CD	1:C:461:ILE:HD11	2.49	0.42
2:D:266:SER:CB	2:D:282:GLN:NE2	2.82	0.42
2:E:166:ILE:O	2:E:170:ILE:HG13	2.18	0.42
1:A:338:ILE:N	1:A:339:PRO:CD	2.83	0.42
1:B:165:GLU:O	1:B:325:PRO:HD2	2.19	0.42
1:B:438:ILE:HD12	1:B:438:ILE:HA	1.87	0.42
2:E:396:LEU:CB	2:E:401:LYS:HG2	2.50	0.42
2:F:251:VAL:HG12	2:F:252:LEU:N	2.35	0.42
1:A:407:GLY:CA	1:A:410:LEU:HD21	2.48	0.42
2:E:32:ILE:O	2:E:33:LEU:CB	2.68	0.42
2:E:231:ARG:O	2:E:234:LEU:N	2.50	0.42
1:A:136:ILE:HD11	2:E:219:TYR:HE2	1.85	0.42
1:B:420:ARG:O	1:B:423:ARG:N	2.50	0.42
1:C:147:GLN:OE1	1:C:438:ILE:HD13	2.19	0.42
2:D:396:LEU:HD23	2:D:396:LEU:HA	1.87	0.42
2:D:412:ARG:C	2:D:414:LEU:N	2.73	0.42
2:F:47:LEU:HD23	2:F:62:ALA:HA	2.01	0.42
2:F:80:ALA:CB	2:F:81:PRO:CD	2.94	0.42
1:B:361:ILE:HD13	1:B:429:LYS:HE2	2.02	0.42
1:B:485:THR:O	1:B:486:ASP:C	2.58	0.42
1:C:30:ARG:HE	1:C:87:ILE:CD1	2.18	0.42
1:C:384:LYS:HB2	1:C:384:LYS:HE3	1.94	0.42
2:D:200:MET:CE	2:D:215:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:97:VAL:HG13	2:E:232:VAL:HG12	2.01	0.42
2:F:423:VAL:O	2:F:423:VAL:HG12	2.20	0.42
1:A:247:PRO:HG2	1:A:274:GLN:NE2	2.35	0.42
1:B:382:ALA:HB1	1:B:442:VAL:HG11	2.02	0.42
1:A:78:ASN:ND2	1:A:80:LYS:HD2	2.34	0.41
1:C:485:THR:O	1:C:486:ASP:C	2.57	0.41
2:D:63:MET:CE	2:D:228:ALA:HA	2.50	0.41
2:D:112:GLN:NE2	2:D:242:TYR:HE1	2.18	0.41
2:E:67:GLU:H	2:E:67:GLU:HG3	1.16	0.41
2:E:320:PRO:HD3	3:G:255:GLN:OE1	2.20	0.41
2:F:81:PRO:O	2:F:82:ILE:C	2.58	0.41
1:A:56:SER:O	1:A:58:GLY:N	2.53	0.41
1:A:99:VAL:HG23	1:A:253:MET:HA	2.01	0.41
1:A:383:MET:O	1:A:386:VAL:HG23	2.19	0.41
2:D:94:ILE:HG22	2:D:102:ILE:HD11	2.01	0.41
2:D:279:VAL:HG12	2:D:279:VAL:O	2.20	0.41
2:D:471:ASP:O	2:D:472:LYS:C	2.58	0.41
2:F:63:MET:HE3	2:F:97:VAL:HG11	2.02	0.41
1:B:75:VAL:HG21	1:B:82:ILE:HD12	2.02	0.41
1:B:433:TYR:C	1:B:435:PRO:HD3	2.40	0.41
2:D:84:ILE:HD12	2:D:95:MET:CE	2.50	0.41
2:E:82:ILE:CG2	2:E:116:ILE:HD13	2.51	0.41
2:E:340:ALA:O	2:E:343:GLY:N	2.42	0.41
2:E:434:LEU:O	2:E:437:THR:HB	2.20	0.41
2:F:38:VAL:HG11	2:F:69:LEU:CD2	2.50	0.41
2:F:400:ASP:O	2:F:404:VAL:HG23	2.19	0.41
1:A:105:GLY:HA2	1:A:226:MET:O	2.21	0.41
1:A:403:PHE:O	1:A:404:ALA:C	2.58	0.41
1:B:78:ASN:ND2	1:B:80:LYS:HE2	2.36	0.41
2:D:35:ALA:HB1	2:D:46:VAL:HG13	2.02	0.41
2:D:401:LYS:H	2:D:401:LYS:HG2	1.72	0.41
2:E:189:ARG:HB2	2:E:192:GLU:HG3	2.02	0.41
2:E:393:MET:HE2	2:E:393:MET:O	2.20	0.41
2:E:397:SER:O	2:E:399:GLU:N	2.54	0.41
2:F:471:ASP:O	2:F:474:ALA:N	2.53	0.41
1:A:383:MET:HG3	1:A:387:ALA:HB2	2.02	0.41
1:B:44:LEU:HB3	1:B:47:VAL:CG2	2.47	0.41
1:C:151:LYS:HE2	1:C:436:MET:SD	2.60	0.41
2:D:86:VAL:HG11	2:D:114:ALA:HB3	2.02	0.41
2:E:77:ASP:C	2:E:79:GLY:H	2.23	0.41
2:E:95:MET:HA	2:E:100:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:183:PHE:HB3	2:E:217:LEU:CD2	2.47	0.41
2:E:185:GLY:HA3	2:E:188:GLU:HG3	2.02	0.41
2:F:434:LEU:O	2:F:438:ILE:HG12	2.21	0.41
3:G:39:LYS:CB	3:G:40:PRO:CD	2.99	0.41
1:A:32:LEU:HD21	1:A:42:HIS:HB2	2.02	0.41
1:A:74:VAL:CG1	1:A:241:PRO:HG3	2.51	0.41
1:A:90:ARG:HB3	1:A:90:ARG:HE	1.73	0.41
1:A:267:ILE:HA	1:A:324:LEU:O	2.20	0.41
1:A:408:SER:O	1:A:409:ASP:HB2	2.20	0.41
1:A:461:ILE:H	1:A:461:ILE:HG12	1.60	0.41
1:B:30:ARG:HA	1:B:86:ASP:O	2.21	0.41
1:B:221:THR:HG22	1:B:222:ASP:N	2.36	0.41
1:B:366:ASN:ND2	1:B:369:LEU:HG	2.36	0.41
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.02	0.41
1:C:373:ARG:NH2	2:D:189:ARG:NH2	2.68	0.41
2:D:112:GLN:NE2	2:D:242:TYR:CE1	2.88	0.41
2:D:203:SER:OG	2:D:205:VAL:HG23	2.20	0.41
2:D:360:PRO:HD3	2:D:368:TYR:CD2	2.56	0.41
2:E:227:GLY:O	2:E:231:ARG:HG2	2.21	0.41
2:E:282:GLN:H	2:E:282:GLN:NE2	2.19	0.41
2:E:388:ILE:HD12	2:E:396:LEU:HD11	2.01	0.41
2:F:430:LYS:HA	2:F:430:LYS:HD3	1.93	0.41
2:F:442:GLN:O	2:F:445:LEU:HB2	2.21	0.41
2:F:445:LEU:HD23	2:F:445:LEU:HA	1.92	0.41
1:B:84:GLU:CD	2:E:56:SER:H	2.23	0.41
1:B:107:VAL:O	1:B:115:ILE:HG12	2.20	0.41
1:B:218:LYS:CG	2:E:128:VAL:HG11	2.48	0.41
1:C:78:ASN:HD21	1:C:80:LYS:HD3	1.85	0.41
1:C:465:GLU:O	1:C:469:LEU:HB2	2.21	0.41
2:D:201:ILE:CD1	2:D:208:LEU:HD11	2.50	0.41
2:D:398:GLU:HA	2:D:401:LYS:CG	2.51	0.41
2:D:402:LEU:O	2:D:406:ARG:HG3	2.21	0.41
2:E:139:VAL:HG21	2:E:348:VAL:HB	2.02	0.41
2:E:387:ILE:HG22	2:E:388:ILE:N	2.36	0.41
3:G:12:SER:O	3:G:16:ILE:HD12	2.20	0.41
1:B:423:ARG:NE	1:B:458:PRO:HD3	2.36	0.41
1:B:430:GLN:HE21	1:B:430:GLN:HB3	1.50	0.41
2:D:13:ILE:HD12	2:D:73:GLN:HB3	2.03	0.41
2:E:387:ILE:HG22	2:E:388:ILE:HD13	2.02	0.41
1:B:383:MET:O	1:B:387:ALA:N	2.53	0.41
1:B:423:ARG:HH21	1:B:458:PRO:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:468:PHE:CZ	1:C:501:VAL:HG12	2.56	0.41
2:D:63:MET:CE	2:D:97:VAL:HG11	2.51	0.41
2:D:475:GLU:OE1	2:D:475:GLU:HA	2.20	0.41
2:E:122:GLU:HB2	2:E:125:GLU:HG3	2.01	0.41
2:E:167:MET:SD	2:E:200:MET:HA	2.61	0.41
2:E:360:PRO:HD3	2:E:368:TYR:CG	2.56	0.41
2:E:452:LEU:HA	2:E:453:PRO:HD3	1.85	0.41
3:G:2:THR:HG22	3:G:4:LYS:H	1.86	0.41
1:A:210:ARG:HH11	1:A:210:ARG:HD2	1.69	0.41
1:A:307:GLU:OE1	2:E:190:THR:HB	2.21	0.41
1:A:422:VAL:O	1:A:426:GLU:HG2	2.21	0.41
1:C:104:LEU:HD21	1:C:257:PHE:CZ	2.56	0.41
1:C:240:ALA:N	1:C:241:PRO:CD	2.84	0.41
1:C:362:ARG:HG3	1:C:362:ARG:HH11	1.86	0.41
1:C:374:VAL:CG1	1:C:378:ALA:HB2	2.51	0.41
1:A:129:VAL:HG12	1:A:249:SER:HA	2.03	0.40
1:A:206:ILE:O	1:A:273:LYS:HD2	2.21	0.40
1:B:99:VAL:HG13	1:B:256:TYR:HB2	2.02	0.40
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.03	0.40
1:C:467:ALA:O	1:C:470:SER:HB2	2.20	0.40
2:D:105:ARG:NH1	2:D:208:LEU:HD23	2.36	0.40
2:D:433:PRO:HG2	2:D:436:GLU:CG	2.45	0.40
2:E:168:GLU:OE1	2:E:420:VAL:HG23	2.22	0.40
2:E:316:ASP:CG	3:G:251:ASN:HB3	2.42	0.40
2:E:412:ARG:NH1	2:E:454:GLU:OE1	2.53	0.40
2:E:416:GLN:NE2	2:E:430:LYS:O	2.54	0.40
2:F:357:ILE:HD13	2:F:357:ILE:HA	1.80	0.40
1:A:69:ASP:O	1:A:70:ASN:HB3	2.21	0.40
1:A:292:GLU:HB2	1:A:294:TYR:HD2	1.86	0.40
1:A:294:TYR:HB2	1:A:337:TYR:CE2	2.54	0.40
1:A:441:GLN:O	1:A:445:ILE:HG12	2.21	0.40
1:B:206:ILE:HA	1:B:234:ALA:O	2.21	0.40
1:C:392:LEU:HD11	2:D:425:THR:HG22	2.03	0.40
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.03	0.40
2:E:33:LEU:HD23	2:E:33:LEU:HA	1.92	0.40
2:E:319:ASP:O	2:E:322:PRO:HD2	2.22	0.40
2:E:359:ASP:HA	2:E:360:PRO:HD2	1.87	0.40
2:F:304:ILE:HD13	2:F:304:ILE:HG21	1.92	0.40
1:A:485:THR:O	1:A:487:GLY:N	2.55	0.40
1:A:492:GLU:C	1:A:494:ASP:N	2.73	0.40
1:A:498:LYS:O	1:A:502:THR:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:HE3	1:B:227:LYS:HZ1	1.87	0.40
1:B:423:ARG:O	1:B:426:GLU:N	2.51	0.40
1:C:105:GLY:N	1:C:229:THR:O	2.41	0.40
2:E:158:ALA:C	2:E:160:VAL:N	2.72	0.40
2:E:165:LEU:HD22	2:E:335:LEU:HD21	2.02	0.40
1:A:268:TYR:HB2	1:A:325:PRO:HA	2.03	0.40
1:A:440:GLU:HG2	1:A:473:ILE:HD11	2.03	0.40
1:A:479:LEU:O	1:A:482:LYS:HB2	2.22	0.40
1:B:488:LYS:HG2	1:B:489:ILE:N	2.37	0.40
1:C:19:ALA:O	1:C:21:THR:HG23	2.21	0.40
1:C:45:ARG:HD3	1:C:45:ARG:HA	1.29	0.40
1:C:151:LYS:HG3	1:C:430:GLN:OE1	2.21	0.40
2:F:228:ALA:O	2:F:232:VAL:HG22	2.21	0.40
1:A:106:ARG:NH2	1:A:119:GLY:O	2.46	0.40
1:A:353:GLU:CD	1:A:366:ASN:HD22	2.24	0.40
2:E:329:LEU:O	2:E:356:ARG:CZ	2.69	0.40

All (58) 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:B:314:ASP:O	1:C:22:SER:C[4_455]	0.42	1.78
1:B:314:ASP:CA	1:C:22:SER:N[4_455]	0.82	1.38
1:B:318:GLY:C	1:C:20:ASP:OD2[4_455]	0.87	1.33
1:B:314:ASP:O	1:C:23:VAL:N[4_455]	0.93	1.27
1:B:314:ASP:OD1	1:C:20:ASP:O[4_455]	0.94	1.26
1:B:314:ASP:CA	1:C:21:THR:C[4_455]	1.04	1.16
1:B:314:ASP:N	1:C:22:SER:N[4_455]	1.12	1.08
1:B:313:ASN:O	1:C:22:SER:CB[4_455]	1.15	1.05
1:B:318:GLY:O	1:C:20:ASP:OD2[4_455]	1.15	1.05
1:B:314:ASP:C	1:C:22:SER:CA[4_455]	1.20	1.00
1:B:318:GLY:CA	1:C:20:ASP:CG[4_455]	1.22	0.98
1:B:124:LYS:NZ	2:F:31:PRO:CB[4_455]	1.27	0.93
1:B:314:ASP:C	1:C:22:SER:C[4_455]	1.29	0.91
1:B:314:ASP:N	1:C:21:THR:C[4_455]	1.30	0.90
1:B:318:GLY:CA	1:C:20:ASP:OD1[4_455]	1.38	0.82
1:B:318:GLY:CA	1:C:20:ASP:OD2[4_455]	1.39	0.81
1:B:314:ASP:CB	1:C:21:THR:C[4_455]	1.44	0.76
1:B:314:ASP:CG	1:C:21:THR:CA[4_455]	1.48	0.72
1:B:314:ASP:CB	1:C:21:THR:CA[4_455]	1.48	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ASP:OD1	1:C:20:ASP:C[4_455]	1.51	0.69
1:B:314:ASP:C	1:C:22:SER:N[4_455]	1.53	0.67
1:B:314:ASP:O	1:C:22:SER:O[4_455]	1.53	0.67
1:B:124:LYS:NZ	2:F:31:PRO:CG[4_455]	1.55	0.65
1:B:318:GLY:N	1:C:22:SER:OG[4_455]	1.57	0.63
1:B:313:ASN:O	1:C:22:SER:OG[4_455]	1.62	0.58
1:B:315:ALA:C	1:C:22:SER:O[4_455]	1.66	0.54
1:B:313:ASN:C	1:C:22:SER:N[4_455]	1.68	0.52
1:B:314:ASP:O	1:C:22:SER:CA[4_455]	1.71	0.49
1:B:315:ALA:N	1:C:22:SER:CA[4_455]	1.73	0.47
1:B:315:ALA:N	1:C:21:THR:O[4_455]	1.75	0.45
1:B:313:ASN:O	1:C:22:SER:CA[4_455]	1.79	0.41
1:B:317:GLY:CA	1:C:23:VAL:CG2[4_455]	1.81	0.39
1:B:314:ASP:C	1:C:23:VAL:N[4_455]	1.84	0.36
1:B:314:ASP:N	1:C:21:THR:CA[4_455]	1.85	0.35
1:B:316:PHE:N	1:C:22:SER:CB[4_455]	1.85	0.35
1:B:314:ASP:N	1:C:21:THR:N[4_455]	1.88	0.32
1:B:314:ASP:CG	1:C:20:ASP:O[4_455]	1.90	0.30
1:B:317:GLY:N	1:C:22:SER:OG[4_455]	1.91	0.29
1:B:314:ASP:C	1:C:21:THR:C[4_455]	1.93	0.27
1:B:311:LYS:NZ	1:C:20:ASP:CB[4_455]	1.96	0.24
1:B:318:GLY:C	1:C:20:ASP:CG[4_455]	1.96	0.24
1:B:313:ASN:O	1:C:22:SER:N[4_455]	1.97	0.23
1:B:314:ASP:CA	1:C:22:SER:CA[4_455]	1.99	0.21
1:B:314:ASP:CB	1:C:21:THR:O[4_455]	2.01	0.19
1:B:314:ASP:CA	1:C:21:THR:CA[4_455]	2.01	0.19
1:B:314:ASP:OD1	1:C:21:THR:N[4_455]	2.02	0.18
1:B:314:ASP:CA	1:C:21:THR:O[4_455]	2.04	0.16
1:B:315:ALA:CA	1:C:22:SER:O[4_455]	2.05	0.15
1:B:316:PHE:N	1:C:22:SER:CA[4_455]	2.06	0.14
1:B:318:GLY:N	1:C:20:ASP:OD1[4_455]	2.06	0.14
1:B:314:ASP:C	1:C:21:THR:O[4_455]	2.08	0.12
1:B:316:PHE:N	1:C:22:SER:O[4_455]	2.09	0.11
1:B:315:ALA:N	1:C:22:SER:C[4_455]	2.11	0.09
1:B:319:GLY:N	1:C:20:ASP:OD2[4_455]	2.12	0.08
1:B:314:ASP:O	1:C:23:VAL:CA[4_455]	2.13	0.07
1:B:314:ASP:OD1	1:C:21:THR:CA[4_455]	2.15	0.05
1:B:318:GLY:O	1:C:20:ASP:CG[4_455]	2.17	0.03
1:B:314:ASP:OD2	1:C:21:THR:CA[4_455]	2.18	0.02

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	485/553 (88%)	443 (91%)	35 (7%)	7 (1%)	11	46
1	B	475/553 (86%)	427 (90%)	41 (9%)	7 (2%)	10	45
1	C	490/553 (89%)	444 (91%)	38 (8%)	8 (2%)	9	44
2	D	465/528 (88%)	419 (90%)	43 (9%)	3 (1%)	25	66
2	E	464/528 (88%)	407 (88%)	48 (10%)	9 (2%)	8	38
2	F	464/528 (88%)	432 (93%)	30 (6%)	2 (0%)	34	72
3	G	134/298 (45%)	130 (97%)	3 (2%)	1 (1%)	22	62
All	All	2977/3541 (84%)	2702 (91%)	238 (8%)	37 (1%)	13	50

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	407	GLY
2	E	393	MET
1	A	57	SER
1	A	405	GLN
1	A	409	ASP
1	B	364	ALA
1	C	332	GLY
1	C	408	SER
1	C	411	ASP
1	C	476	HIS
2	D	28	GLY
2	E	161	GLY
2	E	205	VAL
1	A	364	ALA
1	A	404	ALA
1	B	236	ALA
1	B	452	TYR
2	E	121	PRO

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Mol	Chain	Res	Type
2	E	455	GLN
3	G	72	SER
1	B	411	ASP
1	C	405	GLN
1	C	475	GLN
2	D	474	ALA
2	E	122	GLU
2	F	327	ALA
1	A	484	ARG
1	B	359	LYS
2	E	33	LEU
1	B	458	PRO
1	C	409	ASP
2	E	28	GLY
2	E	279	VAL
1	B	68	PRO
2	F	279	VAL
2	D	279	VAL
1	A	246	ALA

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	393/444 (88%)	351 (89%)	42 (11%)	6	24
1	B	388/444 (87%)	341 (88%)	47 (12%)	5	20
1	C	397/444 (89%)	369 (93%)	28 (7%)	14	39
2	D	377/417 (90%)	346 (92%)	31 (8%)	11	34
2	E	376/417 (90%)	344 (92%)	32 (8%)	10	33
2	F	376/417 (90%)	354 (94%)	22 (6%)	19	45
3	G	116/251 (46%)	110 (95%)	6 (5%)	23	48
All	All	2423/2834 (86%)	2215 (91%)	208 (9%)	10	33

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	40	ARG
1	A	45	ARG
1	A	47	VAL
1	A	48	GLN
1	A	50	GLU
1	A	56	SER
1	A	80	LYS
1	A	94	ILE
1	A	99	VAL
1	A	101	GLU
1	A	102	GLU
1	A	121	ILE
1	A	140	ILE
1	A	143	ARG
1	A	151	LYS
1	A	164	ARG
1	A	173	THR
1	A	188	ARG
1	A	193	THR
1	A	195	GLU
1	A	211	SER
1	A	219	ARG
1	A	256	TYR
1	A	270	ASP
1	A	344	SER
1	A	367	VAL
1	A	371	VAL
1	A	380	THR
1	A	386	VAL
1	A	393	GLU
1	A	409	ASP
1	A	417	LEU
1	A	420	ARG
1	A	436	MET
1	A	444	VAL
1	A	457	GLU
1	A	472	VAL
1	A	474	SER
1	A	479	LEU
1	A	497	LEU
1	A	499	GLU
1	B	38	ILE

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Mol	Chain	Res	Type
1	B	47	VAL
1	B	52	MET
1	B	79	ASP
1	B	80	LYS
1	B	123	SER
1	B	141	SER
1	B	143	ARG
1	B	145	PRO
1	B	164	ARG
1	B	173	THR
1	B	186	GLN
1	B	188	ARG
1	B	189	PHE
1	B	193	THR
1	B	211	SER
1	B	216	LEU
1	B	217	VAL
1	B	218	LYS
1	B	221	THR
1	B	227	LYS
1	B	233	SER
1	B	256	TYR
1	B	270	ASP
1	B	298	VAL
1	B	299	PHE
1	B	335	SER
1	B	349	GLN
1	B	351	PHE
1	B	371	VAL
1	B	374	VAL
1	B	376	SER
1	B	380	THR
1	B	381	ARG
1	B	399	GLU
1	B	416	GLN
1	B	423	ARG
1	B	430	GLN
1	B	442	VAL
1	B	444	VAL
1	B	454	ASP
1	B	474	SER
1	B	479	LEU

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Mol	Chain	Res	Type
1	B	482	LYS
1	B	484	ARG
1	B	490	SER
1	B	505	LEU
1	C	45	ARG
1	C	47	VAL
1	C	56	SER
1	C	63	SER
1	C	64	LEU
1	C	87	ILE
1	C	101	GLU
1	C	164	ARG
1	C	189	PHE
1	C	195	GLU
1	C	208	GLN
1	C	227	LYS
1	C	270	ASP
1	C	282	SER
1	C	298	VAL
1	C	334	VAL
1	C	349	GLN
1	C	399	GLU
1	C	400	VAL
1	C	406	PHE
1	C	440	GLU
1	C	444	VAL
1	C	474	SER
1	C	477	GLN
1	C	479	LEU
1	C	501	VAL
1	C	502	THR
1	C	505	LEU
2	D	27	GLU
2	D	37	GLU
2	D	56	SER
2	D	67	GLU
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	137	ILE
2	D	139	VAL
2	D	166	ILE

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Mol	Chain	Res	Type
2	D	199	GLU
2	D	205	VAL
2	D	223	ASN
2	D	232	VAL
2	D	249	GLN
2	D	266	SER
2	D	282	GLN
2	D	306	SER
2	D	322	PRO
2	D	336	SER
2	D	361	ASN
2	D	365	SER
2	D	388	ILE
2	D	397	SER
2	D	400	ASP
2	D	401	LYS
2	D	405	SER
2	D	423	VAL
2	D	431	LEU
2	D	452	LEU
2	D	475	GLU
2	E	9	THR
2	E	67	GLU
2	E	95	MET
2	E	127	SER
2	E	128	VAL
2	E	132	ILE
2	E	133	LEU
2	E	139	VAL
2	E	148	LYS
2	E	155	PHE
2	E	164	VAL
2	E	194	ASN
2	E	213	SER
2	E	215	VAL
2	E	223	ASN
2	E	257	ASN
2	E	282	GLN
2	E	293	GLN
2	E	297	THR
2	E	306	SER
2	E	358	MET

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Mol	Chain	Res	Type
2	E	365	SER
2	E	385	GLN
2	E	387	ILE
2	E	391	LEU
2	E	393	MET
2	E	394	ASP
2	E	395	GLU
2	E	412	ARG
2	E	431	LEU
2	E	438	ILE
2	E	452	LEU
2	F	10	THR
2	F	27	GLU
2	F	42	GLU
2	F	67	GLU
2	F	95	MET
2	F	112	GLN
2	F	127	SER
2	F	139	VAL
2	F	166	ILE
2	F	191	ARG
2	F	200	MET
2	F	210	ASP
2	F	223	ASN
2	F	232	VAL
2	F	261	PHE
2	F	292	MET
2	F	386	ASP
2	F	387	ILE
2	F	397	SER
2	F	405	SER
2	F	428	LEU
2	F	455	GLN
3	G	35	GLU
3	G	67	LEU
3	G	205	GLN
3	G	212	ILE
3	G	213	ILE
3	G	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	A	396	GLN
1	A	432	GLN
1	B	48	GLN
1	B	349	GLN
1	B	432	GLN
1	C	208	GLN
1	C	260	ASN
1	C	349	GLN
1	C	432	GLN
2	D	130	GLN
2	D	221	GLN
2	D	223	ASN
2	D	282	GLN
2	D	328	HIS
2	D	442	GLN
2	E	39	GLN
2	E	51	GLN
2	E	194	ASN
2	E	223	ASN
2	E	246	GLN
2	E	367	HIS
2	F	39	GLN
2	F	96	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	443	GLN
3	G	82	HIS
3	G	225	GLN
3	G	234	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (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	487/553 (88%)	0.00	7 (1%)	75	66	20, 20, 20, 20	0
1	B	479/553 (86%)	-0.01	2 (0%)	92	87	20, 20, 20, 20	0
1	C	492/553 (88%)	-0.14	1 (0%)	95	93	20, 20, 20, 20	0
2	D	467/528 (88%)	-0.06	3 (0%)	89	84	20, 20, 20, 20	0
2	E	466/528 (88%)	-0.13	3 (0%)	89	84	20, 20, 20, 20	0
2	F	466/528 (88%)	-0.06	4 (0%)	84	77	20, 20, 20, 20	0
3	G	140/298 (46%)	0.48	9 (6%)	19	18	36, 59, 81, 89	0
All	All	2997/3541 (84%)	-0.04	29 (0%)	82	75	20, 20, 20, 89	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	67	LEU	4.0
3	G	202	ARG	3.5
1	A	234	ALA	3.4
1	B	489	ILE	3.2
3	G	69	ILE	3.1
1	A	43	GLY	2.8
3	G	205	GLN	2.7
1	B	510	ALA	2.7
1	A	147	GLN	2.5
2	F	315	ASP	2.4
1	A	233	SER	2.3
2	E	315	ASP	2.3
1	A	42	HIS	2.3
1	C	19	ALA	2.3
2	D	256	ASP	2.2
3	G	208	SER	2.2
2	F	180	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	448	GLU	2.1
2	F	220	GLY	2.1
2	E	451	HIS	2.1
2	E	11	GLY	2.1
3	G	70	GLY	2.1
3	G	71	VAL	2.1
2	F	159	GLY	2.0
3	G	35	GLU	2.0
3	G	48	SER	2.0
1	A	71	VAL	2.0
1	A	69	ASP	2.0
2	D	82	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.