



Full wwPDB X-ray Structure Validation Report i

May 27, 2020 – 12:40 am BST

PDB ID : 6LE5
Title : Crystal structure of the mitochondrial calcium uptake 1 and 2 heterodimer (MICU1-MICU2 heterodimer) in an apo state
Authors : Park, J.; Lee, Y.; Park, T.; Kang, J.Y.; Jin, M.; Yang, J.; Eom, S.H.
Deposited on : 2019-11-24
Resolution : 3.10 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 following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

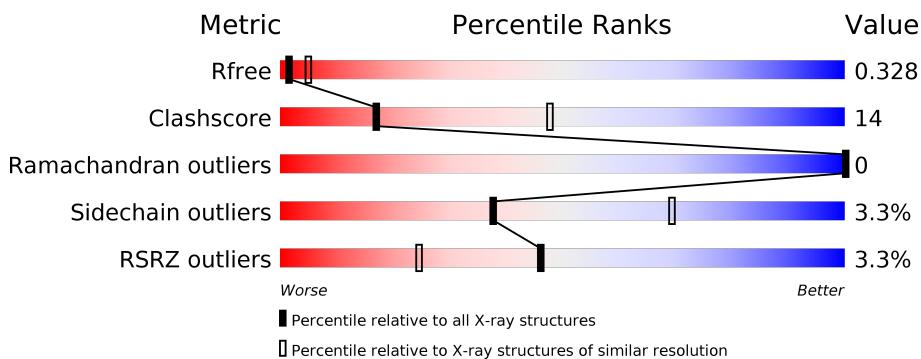
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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.



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Mol	Chain	Length	Quality of chain			
2	F	325	%	63%	21%	• 14%
2	H	325	%	62%	27%	• 10%

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 17392 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 Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1759	1121	300	330	8			
1	D	304	Total	C	N	O	S	0	0	0
			2358	1510	390	444	14			
1	E	304	Total	C	N	O	S	0	0	0
			2380	1521	398	447	14			
1	G	236	Total	C	N	O	S	0	0	0
			1743	1113	296	327	7			

- Molecule 2 is a protein called Calcium uptake protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	Se	0	0	0
			2341	1509	394	422	3	13			
2	C	280	Total	C	N	O	S	Se	0	0	0
			2258	1452	375	416	3	12			
2	F	279	Total	C	N	O	S	Se	0	0	0
			2208	1420	370	404	3	11			
2	H	291	Total	C	N	O	S	Se	0	0	0
			2345	1513	393	423	3	13			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	77	HIS	-	expression tag	UNP Q8IYU8
B	78	HIS	-	expression tag	UNP Q8IYU8
B	79	HIS	-	expression tag	UNP Q8IYU8
B	80	HIS	-	expression tag	UNP Q8IYU8
B	81	HIS	-	expression tag	UNP Q8IYU8
B	82	HIS	-	expression tag	UNP Q8IYU8
B	83	MSE	-	expression tag	UNP Q8IYU8
C	77	HIS	-	expression tag	UNP Q8IYU8

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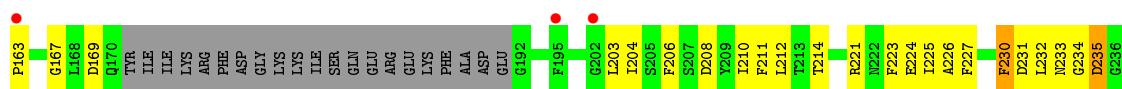
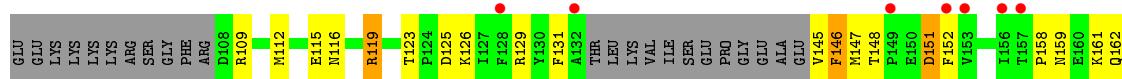
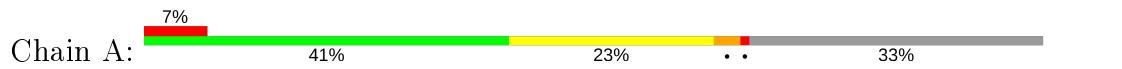
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Chain	Residue	Modelled	Actual	Comment	Reference
C	78	HIS	-	expression tag	UNP Q8IYU8
C	79	HIS	-	expression tag	UNP Q8IYU8
C	80	HIS	-	expression tag	UNP Q8IYU8
C	81	HIS	-	expression tag	UNP Q8IYU8
C	82	HIS	-	expression tag	UNP Q8IYU8
C	83	MSE	-	expression tag	UNP Q8IYU8
F	77	HIS	-	expression tag	UNP Q8IYU8
F	78	HIS	-	expression tag	UNP Q8IYU8
F	79	HIS	-	expression tag	UNP Q8IYU8
F	80	HIS	-	expression tag	UNP Q8IYU8
F	81	HIS	-	expression tag	UNP Q8IYU8
F	82	HIS	-	expression tag	UNP Q8IYU8
F	83	MSE	-	expression tag	UNP Q8IYU8
H	77	HIS	-	expression tag	UNP Q8IYU8
H	78	HIS	-	expression tag	UNP Q8IYU8
H	79	HIS	-	expression tag	UNP Q8IYU8
H	80	HIS	-	expression tag	UNP Q8IYU8
H	81	HIS	-	expression tag	UNP Q8IYU8
H	82	HIS	-	expression tag	UNP Q8IYU8
H	83	MSE	-	expression tag	UNP Q8IYU8

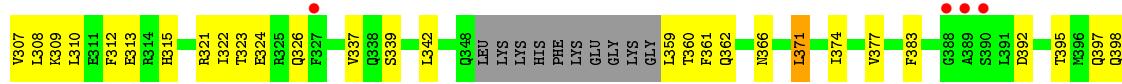
3 Residue-property plots

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

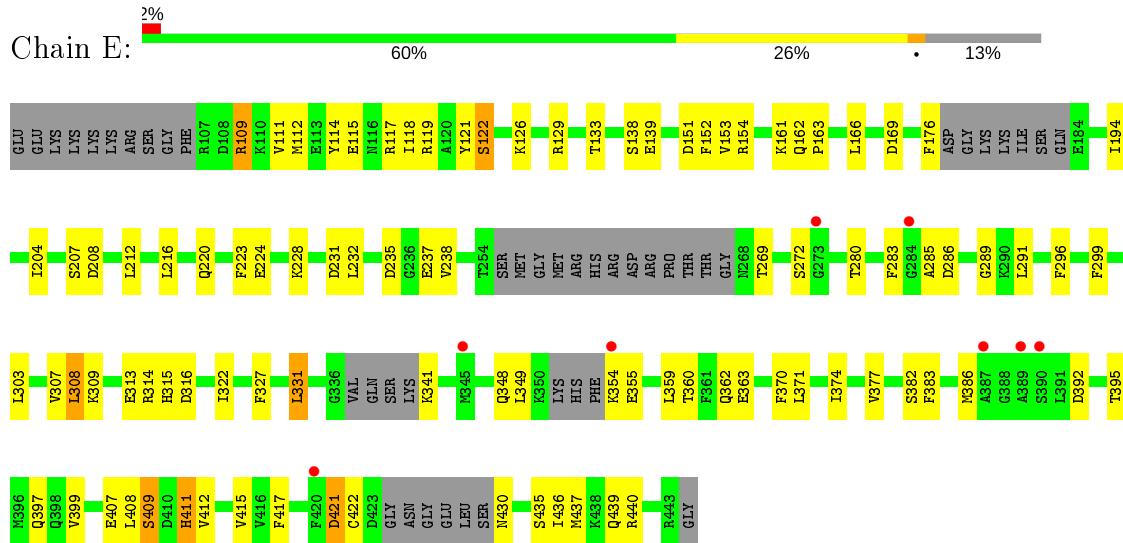
- Molecule 1: Calcium uptake protein 1, mitochondrial



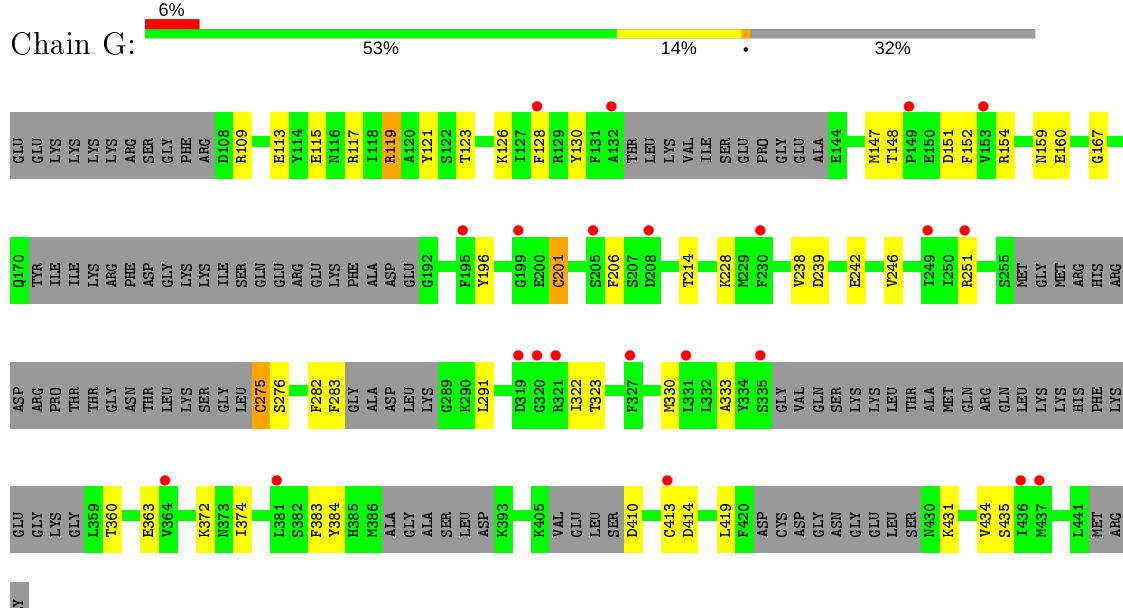
- Molecule 1: Calcium uptake protein 1, mitochondrial



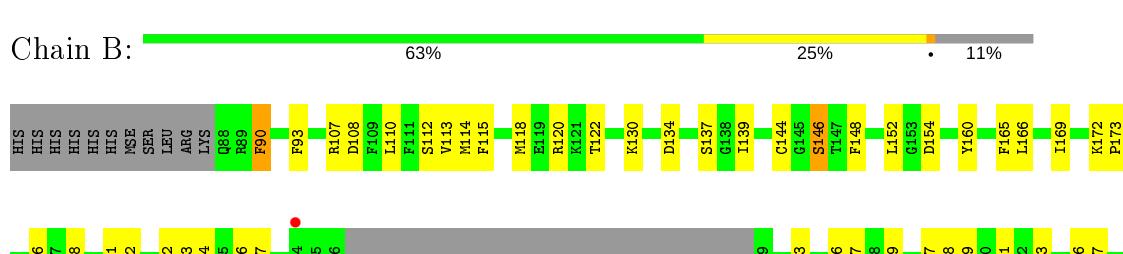
- Molecule 1: Calcium uptake protein 1, mitochondrial



- Molecule 1: Calcium uptake protein 1, mitochondrial



- Molecule 2: Calcium uptake protein 2, mitochondrial

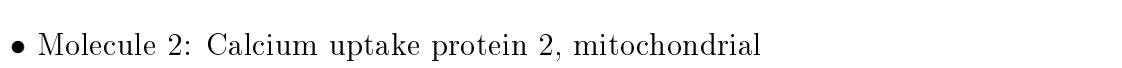


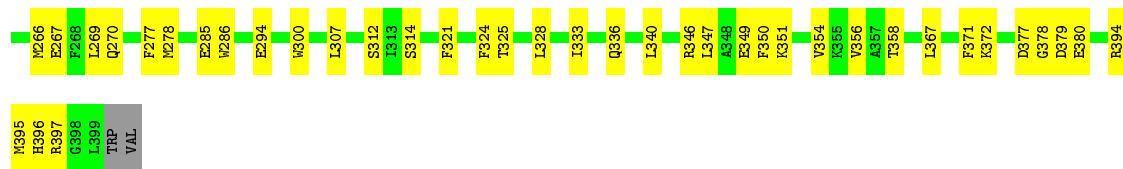


- Molecule 2: Calcium uptake protein 2, mitochondrial



- Molecule 2: Calcium uptake protein 2, mitochondrial





4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.97 Å 173.72 Å 148.00 Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	50.01 – 3.10 49.53 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.01-3.10) 100.0 (49.53-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.63 (at 3.12 Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R , R_{free}	0.293 , 0.332 0.287 , 0.328	Depositor DCC
R_{free} test set	2802 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.0	EDS
L-test for twinning ²	$< L > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17392	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7988e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.45	0/1787	0.95	12/2411 (0.5%)
1	D	0.31	0/2401	0.55	0/3239
1	E	0.33	0/2421	0.60	4/3261 (0.1%)
1	G	0.26	0/1771	0.55	1/2395 (0.0%)
2	B	0.27	0/2379	0.57	1/3166 (0.0%)
2	C	0.29	0/2294	0.59	2/3054 (0.1%)
2	F	0.30	0/2243	0.58	4/2994 (0.1%)
2	H	0.28	0/2383	0.54	0/3172
All	All	0.31	0/17679	0.62	24/23692 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	G	0	1
2	H	0	2
All	All	0	8

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	324	GLU	CB-CA-C	14.64	139.68	110.40
1	G	201	CYS	CB-CA-C	11.90	134.21	110.40
1	A	324	GLU	N-CA-C	-10.77	81.93	111.00
1	A	235	ASP	N-CA-C	-10.15	83.60	111.00
1	A	233	ASN	N-CA-CB	-9.18	94.08	110.60
2	C	300	TRP	CB-CA-C	-8.10	94.20	110.40
2	C	296	LYS	CB-CA-C	-7.59	95.21	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	GLU	C-N-CA	7.42	140.24	121.70
1	A	146	PHE	CB-CA-C	-7.39	95.61	110.40
1	E	232	LEU	CA-CB-CG	7.07	131.57	115.30
1	A	232	LEU	N-CA-C	6.57	128.74	111.00
1	A	233	ASN	CB-CA-C	6.49	123.38	110.40
2	F	343	ARG	N-CA-C	6.47	128.47	111.00
1	A	232	LEU	C-N-CA	6.32	137.51	121.70
2	F	344	PRO	CB-CA-C	-6.24	96.39	112.00
1	A	371	LEU	CA-CB-CG	6.20	129.55	115.30
1	E	139	GLU	CB-CA-C	5.84	122.07	110.40
2	F	340	LEU	CB-CA-C	5.70	121.03	110.20
2	F	93	PHE	CB-CA-C	5.69	121.77	110.40
1	E	139	GLU	N-CA-C	-5.67	95.69	111.00
2	B	146	SER	CB-CA-C	5.24	120.06	110.10
1	A	433	PHE	N-CA-CB	-5.21	101.22	110.60
1	A	203	LEU	CB-CA-C	-5.09	100.53	110.20
1	E	331	LEU	CB-CA-C	-5.09	100.53	110.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ARG	Sidechain
1	A	315	HIS	Peptide
1	A	321	ARG	Peptide
1	A	324	GLU	Peptide
1	A	431	LYS	Mainchain
1	G	119	ARG	Sidechain
2	H	107	ARG	Sidechain
2	H	89	ARG	Sidechain

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	1759	0	1548	79	0
1	D	2358	0	2222	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2380	0	2264	74	0
1	G	1743	0	1529	31	0
2	B	2341	0	2252	70	0
2	C	2258	0	2127	61	0
2	F	2208	0	2044	55	0
2	H	2345	0	2250	62	0
All	All	17392	0	16236	470	0

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 14.

All (470) 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:D:371:LEU:HD21	1:D:437:MET:HB3	1.39	1.02
1:A:147:MET:SD	1:A:152:PHE:HA	2.03	0.97
1:A:119:ARG:HH11	1:A:158:PRO:HA	1.29	0.97
1:G:196:TYR:HA	1:G:201:CYS:O	1.67	0.95
2:B:120:ARG:HE	2:B:122:THR:HG22	1.32	0.91
2:F:180:ALA:O	2:F:184:LEU:HD23	1.77	0.85
2:C:189:ASN:HB3	2:C:191:MSE:HE3	1.60	0.83
1:A:331:LEU:HD22	1:A:437:MET:CE	2.08	0.83
2:H:146:SER:O	2:H:262:GLU:HG2	1.80	0.82
2:B:324:PHE:HA	2:B:358:THR:HG21	1.61	0.81
1:D:397:GLN:NE2	1:D:413:CYS:SG	2.53	0.81
1:A:147:MET:SD	1:A:152:PHE:CA	2.70	0.80
1:E:133:THR:HG23	1:E:151:ASP:OD2	1.82	0.79
1:E:349:LEU:HD13	1:E:354:LYS:HD2	1.64	0.79
2:B:335:MSE:HE1	2:B:345:VAL:HG21	1.66	0.78
1:D:397:GLN:OE1	1:D:408:LEU:HB2	1.83	0.77
2:B:118:MSE:HE3	2:B:120:ARG:HD3	1.65	0.77
2:H:333:ILE:HA	2:H:336:GLN:HB2	1.66	0.76
1:A:147:MET:HB2	1:A:151:ASP:HB3	1.66	0.76
2:C:335:MSE:HE1	2:C:345:VAL:HG11	1.68	0.76
2:H:324:PHE:HA	2:H:358:THR:HG21	1.68	0.75
1:A:148:THR:H	1:A:151:ASP:HB2	1.51	0.75
1:A:146:PHE:CB	1:A:204:ILE:O	2.34	0.74
2:C:265:GLU:O	2:C:269:LEU:HD23	1.87	0.74
1:G:410:ASP:N	1:G:413:CYS:HG	1.84	0.73
2:C:143:GLY:O	2:C:148:PHE:HB2	1.88	0.73
1:A:208:ASP:O	1:A:212:LEU:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:228:LYS:HA	1:E:231:ASP:OD1	1.89	0.71
1:A:331:LEU:HD22	1:A:437:MET:HE3	1.70	0.71
2:C:291:THR:HG21	2:C:390:VAL:HG13	1.73	0.71
2:F:307:LEU:HD11	2:F:369:THR:HG23	1.72	0.70
1:D:374:ILE:HD13	1:D:438:LYS:HG2	1.74	0.69
1:D:339:SER:HA	1:D:342:LEU:HB3	1.74	0.69
1:E:359:LEU:HD12	1:E:363:GLU:OE1	1.92	0.69
1:E:109:ARG:H	1:E:109:ARG:HD3	1.56	0.69
1:D:216:LEU:HD21	1:D:303:LEU:HD22	1.74	0.68
1:G:113:GLU:O	1:G:117:ARG:HG2	1.94	0.68
1:D:366:ASN:HB3	1:D:406:VAL:HG11	1.75	0.68
1:D:119:ARG:NH1	1:D:154:ARG:O	2.27	0.67
2:B:172:LYS:HG3	2:B:173:PRO:HD2	1.76	0.67
1:E:163:PRO:HB2	1:E:166:LEU:HB2	1.75	0.67
1:E:138:SER:HA	1:E:176:PHE:HA	1.77	0.66
2:F:150:ARG:HG2	2:F:266:MSE:HE3	1.77	0.66
2:B:139:ILE:HD11	2:B:233:THR:HA	1.76	0.66
1:A:331:LEU:HD22	1:A:437:MET:HE1	1.76	0.66
2:C:265:GLU:O	2:C:269:LEU:CD2	2.44	0.66
2:C:352:ARG:NH1	1:D:228:LYS:O	2.28	0.66
1:E:119:ARG:NH1	1:E:154:ARG:O	2.29	0.65
2:B:292:ASN:OD1	2:B:296:LYS:NZ	2.28	0.65
1:E:231:ASP:HB2	1:E:237:GLU:O	1.96	0.65
2:H:248:HIS:HB3	2:H:251:GLU:HG2	1.78	0.65
1:D:163:PRO:HB2	1:D:166:LEU:HB2	1.78	0.65
1:A:367:PHE:O	1:A:371:LEU:HB2	1.97	0.65
2:H:104:MSE:HB2	2:H:108:ASP:HB2	1.79	0.64
1:E:238:VAL:O	1:E:291:LEU:N	2.26	0.64
2:H:136:LEU:HD13	2:H:236:MSE:HE2	1.78	0.64
1:A:221:ARG:HH22	2:B:330:ASP:CG	2.02	0.63
1:D:280:THR:HG23	1:D:285:ALA:HA	1.79	0.63
1:A:323:THR:O	1:A:325:ARG:N	2.32	0.63
1:D:231:ASP:HB2	1:D:237:GLU:O	1.98	0.63
2:H:350:PHE:O	2:H:354:VAL:HG23	1.97	0.63
1:E:397:GLN:NE2	1:E:408:LEU:O	2.32	0.63
2:B:146:SER:O	2:B:262:GLU:CD	2.37	0.62
1:A:221:ARG:NH2	2:B:330:ASP:OD1	2.30	0.62
2:C:298:ILE:O	2:C:302:ASN:HB2	1.99	0.62
1:A:116:ASN:OD1	1:A:159:ASN:ND2	2.31	0.62
1:G:147:MET:HE3	1:G:152:PHE:HA	1.82	0.62
1:G:360:THR:HG23	1:G:363:GLU:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:HB2	2:B:341:ALA:HB2	1.80	0.61
2:C:301:LYS:HG3	2:C:304:ARG:HE	1.64	0.61
2:B:166:LEU:HA	2:B:169:ILE:HD12	1.80	0.61
1:A:146:PHE:HB2	1:A:204:ILE:O	2.02	0.60
1:D:374:ILE:HA	1:D:377:VAL:HG12	1.82	0.60
1:A:334:TYR:HD1	1:A:440:ARG:HG2	1.66	0.60
1:G:414:ASP:N	1:G:414:ASP:OD1	2.35	0.60
1:G:384:TYR:CE2	2:H:183:MSE:HG3	2.36	0.60
1:E:314:ARG:O	1:E:314:ARG:HG2	2.00	0.60
1:E:280:THR:HG22	1:E:280:THR:O	2.00	0.60
2:C:343:ARG:HH22	1:D:230:PHE:HE1	1.49	0.60
1:E:315:HIS:HB2	1:E:322:ILE:HD11	1.84	0.60
1:E:407:GLU:OE2	1:E:407:GLU:HA	2.01	0.59
1:A:306:ASP:O	1:A:310:LEU:HG	2.02	0.59
1:E:111:VAL:O	1:E:115:GLU:HG3	2.02	0.59
1:E:435:SER:O	1:E:439:GLN:NE2	2.34	0.59
2:B:120:ARG:HG3	2:B:122:THR:H	1.68	0.59
2:C:93:PHE:CD2	2:C:95:SER:HB2	2.37	0.59
1:A:119:ARG:NH1	1:A:158:PRO:HA	2.08	0.59
1:A:371:LEU:HD11	1:A:437:MET:SD	2.42	0.59
1:D:362:GLN:OE1	1:D:362:GLN:N	2.32	0.59
2:H:113:VAL:HG23	2:H:114:MSE:HG2	1.85	0.58
1:D:133:THR:HG23	1:D:151:ASP:OD2	2.03	0.58
2:C:92:GLN:NE2	2:C:92:GLN:O	2.36	0.58
1:A:282:PHE:HB3	1:A:291:LEU:HD22	1.84	0.58
2:F:93:PHE:CE2	2:F:95:SER:OG	2.50	0.58
1:D:374:ILE:HD11	1:D:434:VAL:HA	1.84	0.58
2:H:377:ASP:N	2:H:378:GLY:HA3	2.18	0.58
2:B:333:ILE:O	2:B:337:MSE:HG2	2.04	0.57
1:A:231:ASP:OD1	1:A:234:GLY:CA	2.52	0.57
1:D:321:ARG:HD3	1:D:321:ARG:N	2.19	0.57
1:A:323:THR:O	1:A:324:GLU:C	2.41	0.57
1:G:119:ARG:HH22	1:G:160:GLU:H	1.51	0.57
2:B:354:VAL:HG11	2:B:362:LEU:HD22	1.87	0.57
2:F:346:ARG:HB2	2:F:349:GLU:OE1	2.04	0.57
1:G:119:ARG:NH1	1:G:154:ARG:O	2.38	0.57
1:A:231:ASP:OD1	1:A:235:ASP:O	2.22	0.57
2:F:292:ASN:HA	2:F:296:LYS:HD3	1.86	0.57
2:B:192:ILE:HG23	2:B:247:LEU:HB3	1.87	0.56
2:H:347:LEU:HA	2:H:371:PHE:CZ	2.40	0.56
2:F:280:LYS:HE3	2:F:311:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:291:THR:HG21	2:F:390:VAL:HG13	1.86	0.56
2:C:295:ASN:O	2:C:299:TYR:CD1	2.59	0.56
1:E:371:LEU:HD11	1:E:440:ARG:HB3	1.87	0.56
2:H:173:PRO:HG2	2:H:395:MSE:HE1	1.87	0.56
1:E:133:THR:HB	1:E:166:LEU:HD13	1.88	0.56
2:B:118:MSE:CE	2:B:120:ARG:HD3	2.35	0.56
1:E:121:TYR:HB2	2:H:294:GLU:HG2	1.86	0.56
1:A:146:PHE:HB2	1:A:204:ILE:H	1.71	0.56
1:E:283:PHE:O	1:E:289:GLY:HA3	2.06	0.56
2:B:166:LEU:HD23	2:B:169:ILE:HD12	1.88	0.55
2:H:139:ILE:HD11	2:H:233:THR:HA	1.88	0.55
2:C:371:PHE:CE2	2:C:382:LEU:HB2	2.42	0.55
2:B:248:HIS:O	2:B:251:GLU:HG2	2.06	0.55
2:B:280:LYS:HG2	2:B:313:ILE:HD11	1.88	0.55
2:B:332:ALA:O	2:B:336:GLN:N	2.33	0.55
1:A:252:SER:CB	2:B:341:ALA:HB2	2.35	0.55
2:F:343:ARG:HH21	2:F:343:ARG:HG2	1.71	0.55
2:H:134:ASP:HA	2:H:137:SER:HB3	1.89	0.55
1:A:147:MET:SD	1:A:152:PHE:CB	2.95	0.55
1:E:133:THR:HG23	1:E:151:ASP:CG	2.27	0.55
2:C:253:ARG:O	2:C:257:GLU:HG2	2.07	0.54
1:G:214:THR:HG21	1:G:251:ARG:HG3	1.87	0.54
1:A:146:PHE:CA	1:A:204:ILE:O	2.55	0.54
2:C:280:LYS:HE2	2:C:365:ASN:HB2	1.89	0.54
2:C:364:ASN:O	2:C:368:ASP:HB3	2.08	0.54
2:H:262:GLU:O	2:H:266:MSE:HG2	2.08	0.54
1:A:334:TYR:HE1	1:A:440:ARG:NH1	2.05	0.54
2:B:114:MSE:HG3	2:B:266:MSE:HE2	1.89	0.54
2:C:109:PHE:O	2:C:113:VAL:HG23	2.08	0.54
1:A:145:VAL:HG12	1:A:145:VAL:O	2.08	0.54
2:F:294:GLU:HG2	1:G:121:TYR:HB2	1.89	0.54
1:E:417:PHE:HB3	1:E:421:ASP:OD1	2.08	0.54
1:E:386:MET:HB3	2:F:203:ILE:HA	1.90	0.54
2:H:172:LYS:HB3	2:H:175:SER:HB2	1.89	0.53
1:A:371:LEU:CD1	1:A:437:MET:SD	2.95	0.53
1:D:236:GLY:O	1:D:293:ILE:N	2.36	0.53
1:E:409:SER:HB3	1:E:412:VAL:HG13	1.90	0.53
2:C:110:LEU:HD13	2:C:266:MSE:SE	2.58	0.53
1:D:109:ARG:O	1:D:112:MET:N	2.41	0.53
1:E:359:LEU:HD11	1:E:412:VAL:HG12	1.91	0.53
1:A:239:ASP:OD2	1:A:242:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PHE:CE1	1:A:437:MET:HG3	2.43	0.53
1:E:112:MET:HE1	1:E:161:LYS:HB2	1.90	0.53
1:A:334:TYR:O	1:A:335:SER:CB	2.56	0.53
1:D:397:GLN:OE1	1:D:397:GLN:HA	2.08	0.53
2:F:150:ARG:CG	2:F:266:MSE:HE3	2.38	0.52
2:F:313:ILE:HG21	2:F:366:ILE:HD11	1.89	0.52
2:B:262:GLU:O	2:B:266:MSE:HG2	2.10	0.52
1:G:115:GLU:O	1:G:119:ARG:HG3	2.09	0.52
1:A:305:HIS:ND1	1:A:365:GLU:OE2	2.34	0.52
1:A:334:TYR:CD1	1:A:440:ARG:HG2	2.44	0.52
1:D:214:THR:HG21	1:D:251:ARG:HB2	1.91	0.52
2:F:321:PHE:O	2:F:325:THR:HG23	2.10	0.52
2:F:104:MSE:HB3	2:F:158:ILE:HB	1.92	0.52
1:A:231:ASP:OD1	1:A:234:GLY:N	2.44	0.51
2:F:111:PHE:HD1	2:F:115:PHE:HE2	1.57	0.51
1:E:153:VAL:HG22	1:E:307:VAL:HG13	1.92	0.51
1:E:228:LYS:O	2:F:352:ARG:NH1	2.38	0.51
1:A:324:GLU:O	1:A:327:PHE:N	2.36	0.51
1:E:395:THR:O	1:E:399:VAL:HG23	2.11	0.51
2:F:110:LEU:HD13	2:F:266:MSE:HE3	1.93	0.51
2:H:351:LYS:HG2	2:H:367:LEU:HD21	1.92	0.51
1:A:146:PHE:CB	1:A:204:ILE:C	2.79	0.51
1:E:327:PHE:CG	1:E:359:LEU:HD23	2.45	0.51
1:E:114:TYR:CZ	1:E:118:ILE:HD11	2.46	0.51
2:B:371:PHE:CE1	2:B:382:LEU:HB2	2.46	0.51
1:A:147:MET:SD	1:A:152:PHE:HB2	2.50	0.50
1:A:147:MET:HB2	1:A:151:ASP:CB	2.39	0.50
1:A:146:PHE:HB3	1:A:204:ILE:C	2.31	0.50
1:E:122:SER:OG	1:E:126:LYS:HD2	2.11	0.50
2:B:335:MSE:CE	2:B:345:VAL:HG21	2.39	0.50
2:B:120:ARG:HG3	2:B:122:THR:N	2.26	0.50
2:F:386:GLU:O	2:F:390:VAL:HG23	2.11	0.50
2:H:97:GLU:HG3	2:H:102:TYR:CE1	2.47	0.50
1:G:228:LYS:HD2	2:H:356:VAL:HG23	1.93	0.50
2:C:187:ASP:HB2	2:C:189:ASN:HD22	1.76	0.50
2:H:146:SER:O	2:H:262:GLU:CG	2.55	0.50
2:C:331:PHE:O	2:C:335:MSE:HG2	2.12	0.50
1:D:286:ASP:N	1:D:286:ASP:OD1	2.37	0.50
1:E:129:ARG:HD3	1:E:269:THR:HA	1.94	0.50
1:E:370:PHE:CE1	1:E:377:VAL:HG21	2.47	0.50
2:H:114:MSE:HG3	2:H:266:MSE:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PHE:C	1:A:433:PHE:CD1	2.85	0.50
2:B:192:ILE:HG13	2:B:196:GLU:HB2	1.93	0.50
1:D:151:ASP:OD1	1:D:154:ARG:NH2	2.32	0.50
1:D:409:SER:O	1:D:412:VAL:HG22	2.11	0.50
1:G:128:PHE:CE1	1:G:147:MET:HG3	2.47	0.50
1:A:231:ASP:OD1	1:A:235:ASP:N	2.45	0.49
1:A:224:GLU:HA	1:A:293:ILE:HD12	1.94	0.49
2:C:167:LEU:O	2:C:171:THR:HG22	2.11	0.49
2:B:335:MSE:HE1	2:B:345:VAL:HG11	1.93	0.49
2:C:179:VAL:O	2:C:183:MSE:HG2	2.12	0.49
2:H:107:ARG:NH2	2:H:154:ASP:OD2	2.46	0.49
2:H:286:TRP:O	2:H:394:ARG:NH1	2.45	0.49
2:C:295:ASN:HB2	2:C:299:TYR:CE1	2.47	0.49
2:C:97:GLU:HB3	2:C:103:TYR:HB2	1.94	0.49
1:D:238:VAL:O	1:D:291:LEU:N	2.27	0.49
1:A:123:THR:HG23	1:A:126:LYS:H	1.77	0.49
2:B:93:PHE:O	2:B:120:ARG:NH2	2.46	0.49
2:F:110:LEU:HD13	2:F:266:MSE:CE	2.42	0.49
2:H:195:ARG:NH1	2:H:196:GLU:OE2	2.46	0.49
1:A:158:PRO:HG2	1:A:333:ALA:O	2.13	0.49
2:C:313:ILE:HG21	2:C:366:ILE:HD11	1.95	0.49
1:D:312:PHE:CE2	1:D:361:PHE:HB2	2.47	0.49
2:F:148:PHE:O	2:F:152:LEU:HG	2.13	0.49
1:E:348:GLN:O	1:E:349:LEU:HD23	2.13	0.48
2:C:295:ASN:O	2:C:299:TYR:HD1	1.96	0.48
1:D:291:LEU:HD22	1:D:296:PHE:HB2	1.94	0.48
1:A:237:GLU:HA	1:A:292:THR:HA	1.96	0.48
2:F:325:THR:HG22	2:F:391:LEU:HD21	1.95	0.48
2:B:113:VAL:HG21	2:B:263:ILE:HD12	1.96	0.48
2:F:199:LYS:O	2:F:203:ILE:N	2.42	0.48
1:G:242:GLU:O	1:G:246:VAL:HG23	2.13	0.48
1:G:330:MET:HA	1:G:333:ALA:HB2	1.96	0.48
2:H:336:GLN:O	2:H:340:LEU:N	2.41	0.48
1:D:360:THR:OG1	1:D:361:PHE:N	2.46	0.48
1:A:433:PHE:HE1	1:A:437:MET:HG3	1.77	0.48
2:F:343:ARG:NH2	2:F:343:ARG:HG2	2.28	0.48
2:H:321:PHE:O	2:H:325:THR:HG23	2.14	0.48
1:D:323:THR:HB	1:D:326:GLN:HB2	1.94	0.48
1:E:194:ILE:HD11	1:E:299:PHE:CE1	2.49	0.48
1:G:128:PHE:HE1	1:G:147:MET:HG3	1.79	0.48
2:B:321:PHE:O	2:B:325:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:352:ARG:O	2:C:356:VAL:HG12	2.14	0.47
2:F:110:LEU:O	2:F:114:MSE:HG2	2.14	0.47
1:D:150:GLU:N	1:D:150:GLU:OE1	2.42	0.47
1:E:440:ARG:HA	1:E:440:ARG:HD2	1.65	0.47
2:H:89:ARG:NH2	2:H:112:SER:O	2.47	0.47
2:F:107:ARG:O	2:F:111:PHE:CD2	2.67	0.47
2:F:241:LYS:H	2:F:241:LYS:HD2	1.79	0.47
2:F:285:GLU:HA	2:F:300:TRP:CH2	2.49	0.47
2:C:137:SER:O	2:C:140:GLN:HG2	2.13	0.47
2:B:115:PHE:CD2	2:B:118:MSE:SE	3.17	0.47
2:F:369:THR:O	2:F:373:ILE:HG13	2.15	0.47
1:D:309:LYS:O	1:D:313:GLU:HG2	2.15	0.47
1:E:207:SER:HB3	1:E:272:SER:HB2	1.96	0.47
2:F:374:PHE:HE2	2:F:390:VAL:HG21	1.78	0.47
1:G:148:THR:HG23	1:G:151:ASP:H	1.80	0.47
2:H:186:THR:OG1	2:H:187:ASP:N	2.47	0.47
1:A:119:ARG:HH11	1:A:158:PRO:CA	2.16	0.47
2:B:90:PHE:CZ	2:B:160:TYR:HB2	2.50	0.47
2:B:236:MSE:HE2	2:B:236:MSE:HB3	1.86	0.47
2:F:113:VAL:HG12	2:F:397:ARG:NH1	2.30	0.47
2:B:114:MSE:HB3	2:B:114:MSE:HE3	1.85	0.47
2:B:148:PHE:CZ	2:B:152:LEU:HD11	2.49	0.47
1:D:274:LEU:O	1:D:275:CYS:SG	2.73	0.47
2:H:192:ILE:HG23	2:H:247:LEU:HB3	1.97	0.46
2:C:118:MSE:O	2:C:121:LYS:NZ	2.48	0.46
1:D:227:PHE:CE2	1:D:238:VAL:HG12	2.51	0.46
2:H:163:TYR:CZ	2:H:167:LEU:HD11	2.49	0.46
2:B:115:PHE:HD2	2:B:118:MSE:SE	2.48	0.46
2:B:165:PHE:CE2	2:B:169:ILE:HD11	2.50	0.46
2:B:327:HIS:HB2	2:B:358:THR:HG22	1.97	0.46
2:B:290:PHE:CZ	2:B:397:ARG:HB3	2.51	0.46
1:D:211:PHE:O	1:D:215:VAL:HG23	2.15	0.46
2:F:127:LEU:O	2:F:131:ASP:N	2.48	0.46
1:A:396:MET:O	1:A:399:VAL:N	2.48	0.46
2:B:337:MSE:O	2:B:340:LEU:O	2.33	0.46
2:C:271:PHE:HB2	2:C:278:MSE:HE2	1.96	0.46
2:F:150:ARG:HG2	2:F:266:MSE:CE	2.45	0.46
2:F:232:THR:O	2:F:236:MSE:HG3	2.14	0.46
1:A:242:GLU:O	1:A:246:VAL:HG23	2.15	0.46
2:H:165:PHE:CE2	2:H:169:ILE:HD11	2.50	0.46
2:H:259:LEU:O	2:H:262:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:GLN:HE22	2:B:340:LEU:HB2	1.81	0.46
1:A:309:LYS:O	1:A:313:GLU:CB	2.63	0.46
1:E:382:SER:O	1:E:386:MET:HG2	2.16	0.46
1:E:436:ILE:HA	1:E:439:GLN:HE21	1.81	0.46
2:F:134:ASP:OD2	2:F:155:LYS:HG2	2.15	0.46
1:G:130:TYR:HA	1:G:167:GLY:O	2.15	0.46
1:A:147:MET:N	1:A:204:ILE:O	2.49	0.46
2:B:341:ALA:O	2:B:342:HIS:C	2.53	0.46
2:C:113:VAL:O	2:C:397:ARG:HD3	2.15	0.46
1:G:383:PHE:HB2	2:H:183:MSE:SE	2.65	0.46
1:D:153:VAL:HG21	1:D:310:LEU:HB2	1.98	0.46
2:F:338:PHE:O	2:F:342:HIS:O	2.34	0.46
1:D:153:VAL:HG22	1:D:307:VAL:HG13	1.98	0.45
2:C:247:LEU:HD11	2:C:252:PHE:HB2	1.99	0.45
1:E:360:THR:HG22	1:E:363:GLU:OE1	2.15	0.45
1:A:221:ARG:O	1:A:225:ILE:HG13	2.17	0.45
1:D:374:ILE:HD12	1:D:437:MET:HB2	1.98	0.45
1:E:283:PHE:O	1:E:289:GLY:CA	2.64	0.45
1:A:167:GLY:O	1:A:169:ASP:N	2.50	0.45
2:C:162:GLU:CD	2:C:232:THR:HG1	2.18	0.45
1:D:227:PHE:CD2	1:D:293:ILE:HG12	2.51	0.45
1:E:417:PHE:O	1:E:421:ASP:OD1	2.35	0.45
2:F:197:PHE:O	2:F:201:GLN:HG3	2.16	0.45
2:H:89:ARG:NH1	2:H:93:PHE:HE2	2.13	0.45
1:D:322:ILE:N	1:D:359:LEU:O	2.50	0.45
1:A:162:GLN:HB3	1:A:163:PRO:HD2	1.99	0.45
2:H:379:ASP:O	2:H:380:GLU:HG2	2.17	0.45
2:B:192:ILE:CG2	2:B:247:LEU:HB3	2.46	0.45
2:C:278:MSE:O	2:C:312:SER:OG	2.29	0.45
1:E:383:PHE:HB3	2:F:183:MSE:SE	2.67	0.45
2:B:110:LEU:HD22	2:B:266:MSE:SE	2.67	0.45
2:B:306:LYS:O	2:B:372:LYS:HD2	2.16	0.45
2:C:269:LEU:HD22	2:C:269:LEU:N	2.32	0.45
1:A:227:PHE:HD2	1:A:293:ILE:HB	1.81	0.44
1:A:224:GLU:HG2	1:A:293:ILE:HD13	2.00	0.44
1:D:442:MET:O	1:D:443:ARG:HG2	2.17	0.44
1:E:129:ARG:HD2	1:E:169:ASP:OD1	2.17	0.44
2:C:156:GLY:HA2	2:C:233:THR:HG21	1.98	0.44
2:C:170:LEU:HD21	2:C:259:LEU:HG	2.00	0.44
1:E:308:LEU:HD23	1:E:308:LEU:HA	1.81	0.44
1:E:355:GLU:O	1:E:355:GLU:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:431:LYS:O	1:G:435:SER:OG	2.35	0.44
1:A:119:ARG:HH21	1:A:131:PHE:HZ	1.65	0.44
2:B:178:HIS:NE2	2:B:182:LYS:HE2	2.32	0.44
1:D:136:VAL:HA	1:D:174:LYS:HB2	1.98	0.44
2:F:341:ALA:O	2:F:342:HIS:C	2.53	0.44
1:G:148:THR:O	1:G:151:ASP:N	2.51	0.44
2:C:301:LYS:HG2	2:C:304:ARG:HH21	1.81	0.44
1:D:194:ILE:O	1:D:197:THR:HG23	2.18	0.44
1:E:151:ASP:OD1	1:E:154:ARG:NH2	2.35	0.44
2:H:148:PHE:CZ	2:H:152:LEU:HD11	2.51	0.44
2:B:172:LYS:NZ	2:B:176:GLY:O	2.51	0.44
2:H:192:ILE:HD11	2:H:197:PHE:HA	2.00	0.44
2:H:285:GLU:HA	2:H:300:TRP:HH2	1.83	0.44
1:A:210:ILE:O	1:A:214:THR:HG23	2.18	0.44
2:C:338:PHE:CE2	2:C:349:GLU:HG2	2.52	0.44
2:H:266:MSE:O	2:H:270:GLN:HG2	2.18	0.44
2:B:351:LYS:HG2	2:B:367:LEU:HD21	2.00	0.44
1:D:200:GLU:O	1:D:202:GLY:N	2.50	0.44
2:F:249:TYR:O	2:F:253:ARG:N	2.44	0.44
2:H:168:THR:HG21	2:H:204:ILE:HG21	2.00	0.44
1:A:278:LEU:HD12	1:A:281:TYR:HB3	2.00	0.44
1:A:400:ALA:HA	1:A:404:ALA:HB3	2.00	0.44
1:G:123:THR:HG23	1:G:126:LYS:H	1.83	0.44
1:E:223:PHE:CD2	1:E:296:PHE:HE2	2.35	0.43
1:E:411:HIS:O	1:E:415:VAL:HG23	2.18	0.43
1:G:147:MET:CE	1:G:152:PHE:HA	2.46	0.43
2:H:127:LEU:HD21	2:H:132:ILE:HG23	1.99	0.43
1:A:371:LEU:HG	1:A:437:MET:SD	2.58	0.43
1:D:227:PHE:CE1	1:D:246:VAL:HG11	2.54	0.43
1:A:116:ASN:N	1:A:116:ASN:HD22	2.14	0.43
2:C:159:SER:OG	2:C:162:GLU:HG3	2.18	0.43
1:E:371:LEU:HD21	1:E:437:MET:O	2.17	0.43
2:F:279:ARG:HB3	2:F:282:ASP:OD2	2.19	0.43
2:B:93:PHE:CE2	2:B:112:SER:HA	2.53	0.43
2:C:114:MSE:HE1	2:C:266:MSE:SE	2.68	0.43
2:B:181:PHE:CG	2:B:249:TYR:HD1	2.37	0.43
1:E:231:ASP:OD2	1:E:235:ASP:O	2.36	0.43
2:H:107:ARG:HD2	2:H:111:PHE:CZ	2.54	0.43
2:B:139:ILE:HD12	2:B:236:MSE:HB2	2.00	0.43
2:C:148:PHE:O	2:C:149:PHE:HB2	2.18	0.43
2:F:294:GLU:H	2:F:294:GLU:CD	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:271:PHE:CE1	2:C:286:TRP:HD1	2.36	0.43
1:D:208:ASP:O	1:D:212:LEU:HG	2.18	0.43
1:D:395:THR:O	1:D:399:VAL:HG23	2.19	0.43
2:F:169:ILE:HG23	2:F:256:MSE:HG2	2.00	0.43
1:E:133:THR:CG2	1:E:151:ASP:OD2	2.60	0.43
2:H:267:GLU:OE2	2:H:394:ARG:NH2	2.51	0.43
2:B:347:LEU:HA	2:B:371:PHE:CZ	2.54	0.43
2:C:352:ARG:HH12	1:D:234:GLY:HA2	1.82	0.43
1:E:360:THR:HG22	1:E:363:GLU:CD	2.38	0.43
2:H:135:THR:HG23	2:H:233:THR:HG23	2.00	0.43
1:D:188:PHE:HD2	1:D:201:CYS:O	2.02	0.43
2:H:346:ARG:HB2	2:H:349:GLU:OE1	2.19	0.43
1:A:321:ARG:O	1:A:323:THR:CB	2.67	0.42
1:A:372:LYS:HA	1:A:372:LYS:HE2	2.00	0.42
2:C:192:ILE:HG12	2:C:193:GLU:H	1.84	0.42
2:C:292:ASN:HA	2:C:296:LYS:HE3	2.00	0.42
1:D:392:ASP:N	1:D:395:THR:OG1	2.50	0.42
1:E:152:PHE:HB2	1:E:204:ILE:HD12	2.01	0.42
1:E:154:ARG:NE	1:E:162:GLN:OE1	2.46	0.42
1:E:327:PHE:CZ	1:E:331:LEU:HD11	2.54	0.42
2:B:338:PHE:HB3	2:B:343:ARG:O	2.18	0.42
1:D:220:GLN:O	1:D:224:GLU:HG3	2.19	0.42
1:E:117:ARG:HB3	2:H:294:GLU:HG3	2.02	0.42
2:H:87:LYS:C	2:H:89:ARG:H	2.21	0.42
2:B:107:ARG:NH1	2:B:154:ASP:OD2	2.53	0.42
2:B:134:ASP:HA	2:B:137:SER:HB3	2.01	0.42
1:D:398:GLN:HA	1:D:398:GLN:OE1	2.19	0.42
1:G:239:ASP:H	1:G:242:GLU:HB2	1.84	0.42
1:A:239:ASP:CG	1:A:242:GLU:HG3	2.40	0.42
1:D:133:THR:HG23	1:D:151:ASP:CG	2.39	0.42
2:F:170:LEU:HD21	2:F:259:LEU:HG	2.02	0.42
2:H:185:ASP:OD2	2:H:196:GLU:HG3	2.20	0.42
2:C:346:ARG:NH1	2:C:380:GLU:O	2.53	0.42
1:D:324:GLU:H	1:D:324:GLU:HG2	1.62	0.42
2:C:244:GLN:OE1	1:E:286:ASP:HB2	2.19	0.42
1:E:377:VAL:HG23	1:E:399:VAL:HG12	2.01	0.42
1:E:409:SER:O	1:E:412:VAL:HG22	2.20	0.42
2:B:146:SER:O	2:B:262:GLU:CG	2.68	0.42
2:C:285:GLU:HA	2:C:300:TRP:CH2	2.55	0.42
2:H:89:ARG:NH1	2:H:93:PHE:CE2	2.87	0.42
2:B:114:MSE:SE	2:B:266:MSE:HE2	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:CYS:HA	2:B:237:ARG:HH21	1.83	0.42
2:B:169:ILE:HG23	2:B:256:MSE:HE3	2.02	0.42
2:C:192:ILE:HG22	2:C:247:LEU:HB3	2.02	0.42
1:D:337:VAL:HG13	1:D:337:VAL:O	2.19	0.42
2:H:166:LEU:HD23	2:H:169:ILE:HD12	2.01	0.42
2:H:197:PHE:HB2	2:H:239:PHE:CZ	2.54	0.42
2:H:307:LEU:HA	2:H:372:LYS:HZ2	1.84	0.42
1:A:313:GLU:O	1:A:317:PRO:HG3	2.20	0.42
2:B:107:ARG:NH2	2:C:279:ARG:HB2	2.34	0.42
2:C:269:LEU:H	2:C:269:LEU:HD22	1.85	0.42
2:C:374:PHE:HE2	2:C:390:VAL:HG21	1.84	0.42
1:E:408:LEU:HD23	1:E:408:LEU:HA	1.84	0.42
1:E:392:ASP:HA	1:E:417:PHE:CZ	2.55	0.42
1:G:275:CYS:HB2	1:G:276:SER:H	1.58	0.42
1:A:125:ASP:O	1:A:129:ARG:HG3	2.20	0.41
2:B:108:ASP:O	2:B:112:SER:OG	2.28	0.41
1:E:280:THR:HG23	1:E:285:ALA:HA	2.02	0.41
1:E:315:HIS:O	1:E:316:ASP:HB2	2.20	0.41
2:C:162:GLU:HB3	2:C:234:LEU:HD12	2.02	0.41
1:D:315:HIS:HB3	1:D:326:GLN:OE1	2.20	0.41
2:F:236:MSE:HA	2:F:240:GLY:O	2.20	0.41
2:F:321:PHE:HA	2:F:362:LEU:HD21	2.02	0.41
2:H:113:VAL:HG21	2:H:263:ILE:HD12	2.02	0.41
2:B:193:GLU:HG3	2:B:194:LYS:N	2.34	0.41
1:E:362:GLN:OE1	1:E:362:GLN:N	2.43	0.41
2:H:114:MSE:HE2	2:H:270:GLN:HG3	2.03	0.41
2:C:232:THR:O	2:C:236:MSE:HG3	2.20	0.41
2:F:338:PHE:CE2	2:F:349:GLU:HG2	2.55	0.41
1:G:238:VAL:O	1:G:291:LEU:N	2.35	0.41
1:A:372:LYS:O	1:A:374:ILE:HG22	2.21	0.41
2:F:163:TYR:CZ	2:F:167:LEU:HD11	2.56	0.41
2:C:352:ARG:HH22	1:D:233:ASN:C	2.23	0.41
1:E:216:LEU:HD21	1:E:303:LEU:HD22	2.03	0.41
1:E:309:LYS:O	1:E:313:GLU:HG2	2.21	0.41
2:F:352:ARG:O	2:F:356:VAL:HG23	2.21	0.41
2:F:380:GLU:HG3	2:F:380:GLU:O	2.20	0.41
1:G:322:ILE:O	1:G:323:THR:HG22	2.20	0.41
2:H:247:LEU:HD12	2:H:251:GLU:OE2	2.21	0.41
1:A:115:GLU:OE1	1:A:161:LYS:HA	2.20	0.41
1:A:226:ALA:O	1:A:230:PHE:HD1	2.03	0.41
2:C:233:THR:O	2:C:237:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:191:MSE:HB3	2:C:191:MSE:HE2	1.93	0.41
1:E:280:THR:CG2	1:E:280:THR:O	2.68	0.41
2:H:294:GLU:CD	2:H:294:GLU:H	2.24	0.41
1:A:368:PHE:HA	1:A:371:LEU:HB3	2.01	0.41
1:D:138:SER:H	1:D:175:ARG:HB2	1.86	0.41
2:F:343:ARG:O	2:F:343:ARG:HG2	2.21	0.41
2:H:171:THR:HG23	2:H:396:HIS:HA	2.01	0.41
2:H:259:LEU:O	2:H:263:ILE:HG12	2.21	0.41
2:C:163:TYR:CZ	2:C:167:LEU:HD11	2.56	0.41
2:C:199:LYS:HD2	2:C:199:LYS:HA	1.86	0.41
1:E:228:LYS:HB3	2:F:356:VAL:HG22	2.02	0.41
1:A:109:ARG:HD2	1:A:112:MET:SD	2.60	0.40
2:B:197:PHE:HB2	2:B:239:PHE:CZ	2.56	0.40
1:E:208:ASP:O	1:E:212:LEU:HG	2.20	0.40
1:E:220:GLN:O	1:E:224:GLU:HG3	2.21	0.40
2:F:279:ARG:O	2:F:282:ASP:HB2	2.21	0.40
1:G:282:PHE:CG	1:G:291:LEU:HD22	2.56	0.40
1:G:374:ILE:HD11	1:G:434:VAL:HG13	2.02	0.40
1:A:316:ASP:CB	1:A:326:GLN:HE22	2.34	0.40
2:B:130:LYS:HB3	2:B:130:LYS:HE3	1.82	0.40
2:B:165:PHE:O	2:B:169:ILE:HG13	2.21	0.40
2:H:277:PHE:HB3	2:H:312:SER:HB2	2.03	0.40
2:B:253:ARG:O	2:B:257:GLU:HG2	2.21	0.40
2:B:353:ALA:HA	2:B:356:VAL:HG12	2.02	0.40
1:G:159:ASN:O	1:G:160:GLU:HG2	2.20	0.40
2:B:107:ARG:NH2	2:B:154:ASP:OD2	2.54	0.40
1:D:441:LEU:HA	1:D:441:LEU:HD23	1.98	0.40
1:E:374:ILE:HA	1:E:377:VAL:HG12	2.03	0.40
2:F:313:ILE:HG23	2:F:317:GLU:HB2	2.02	0.40
2:H:269:LEU:HA	2:H:269:LEU:HD13	1.85	0.40
1:A:227:PHE:CD2	1:A:293:ILE:HB	2.55	0.40
2:F:162:GLU:OE2	2:F:232:THR:HG21	2.22	0.40
2:H:146:SER:C	2:H:262:GLU:HG2	2.41	0.40

There are no symmetry-related clashes.

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	214/348 (62%)	189 (88%)	25 (12%)	0	100 100
1	D	294/348 (84%)	274 (93%)	20 (7%)	0	100 100
1	E	292/348 (84%)	276 (94%)	16 (6%)	0	100 100
1	G	218/348 (63%)	192 (88%)	26 (12%)	0	100 100
2	B	285/325 (88%)	277 (97%)	8 (3%)	0	100 100
2	C	272/325 (84%)	259 (95%)	13 (5%)	0	100 100
2	F	271/325 (83%)	260 (96%)	11 (4%)	0	100 100
2	H	287/325 (88%)	275 (96%)	12 (4%)	0	100 100
All	All	2133/2692 (79%)	2002 (94%)	131 (6%)	0	100 100

There are no Ramachandran outliers to report.

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	166/309 (54%)	154 (93%)	12 (7%)	14 44
1	D	243/309 (79%)	232 (96%)	11 (4%)	27 60
1	E	247/309 (80%)	238 (96%)	9 (4%)	35 67
1	G	162/309 (52%)	156 (96%)	6 (4%)	34 66
2	B	244/282 (86%)	243 (100%)	1 (0%)	91 96
2	C	235/282 (83%)	228 (97%)	7 (3%)	41 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	223/282 (79%)	216 (97%)	7 (3%)	40 70
2	H	243/282 (86%)	237 (98%)	6 (2%)	47 75
All	All	1763/2364 (75%)	1704 (97%)	59 (3%)	38 69

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	ASP
1	A	206	PHE
1	A	211	PHE
1	A	223	PHE
1	A	230	PHE
1	A	370	PHE
1	A	372	LYS
1	A	373	ASN
1	A	384	TYR
1	A	433	PHE
1	A	436	ILE
1	A	440	ARG
2	B	90	PHE
2	C	92	GLN
2	C	93	PHE
2	C	99	GLU
2	C	272	SER
2	C	312	SER
2	C	328	LEU
2	C	380	GLU
1	D	109	ARG
1	D	147	MET
1	D	177	ASP
1	D	235	ASP
1	D	308	LEU
1	D	371	LEU
1	D	383	PHE
1	D	409	SER
1	D	435	SER
1	D	440	ARG
1	D	443	ARG
1	E	109	ARG
1	E	122	SER
1	E	308	LEU

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Mol	Chain	Res	Type
1	E	341	LYS
1	E	409	SER
1	E	411	HIS
1	E	421	ASP
1	E	422	CYS
1	E	430	ASN
2	F	92	GLN
2	F	93	PHE
2	F	95	SER
2	F	115	PHE
2	F	181	PHE
2	F	241	LYS
2	F	346	ARG
1	G	109	ARG
1	G	206	PHE
1	G	275	CYS
1	G	283	PHE
1	G	372	LYS
1	G	419	LEU
2	H	87	LYS
2	H	193	GLU
2	H	278	MSE
2	H	314	SER
2	H	328	LEU
2	H	397	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	159	ASN
1	A	253	GLN
1	A	300	GLN
1	A	315	HIS
1	A	326	GLN
1	D	397	GLN
1	G	385	HIS

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 carbohydrates 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	234/348 (67%)	0.53	24 (10%) 6 2	68, 102, 136, 158	0
1	D	304/348 (87%)	0.17	11 (3%) 42 22	38, 82, 120, 130	0
1	E	304/348 (87%)	0.06	8 (2%) 56 33	30, 67, 116, 131	0
1	G	236/348 (67%)	0.45	22 (9%) 8 3	68, 103, 138, 156	0
2	B	276/325 (84%)	-0.06	1 (0%) 92 84	32, 61, 97, 115	0
2	C	267/325 (82%)	-0.02	2 (0%) 87 75	37, 69, 102, 128	0
2	F	266/325 (81%)	-0.01	2 (0%) 86 72	31, 68, 107, 124	0
2	H	278/325 (85%)	-0.10	2 (0%) 87 75	31, 56, 97, 121	0
All	All	2165/2692 (80%)	0.11	72 (3%) 46 24	30, 75, 122, 158	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	GLY	6.7
1	D	420	PHE	4.6
1	G	319	ASP	4.6
1	E	345	MET	3.9
1	A	128	PHE	3.9
1	G	195	PHE	3.8
1	D	419	LEU	3.8
1	G	230	PHE	3.7
2	F	176	GLY	3.7
1	D	389	ALA	3.6
1	G	249	ILE	3.6
1	E	387	ALA	3.5
1	G	132	ALA	3.4
1	D	429	SER	3.4
1	A	375	ASN	3.4
1	A	202	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	175	SER	3.4
1	A	149	PRO	3.4
1	D	390	SER	3.3
1	G	199	GLY	3.3
1	A	132	ALA	3.2
1	G	436	ILE	3.2
1	A	152	PHE	3.1
1	A	157	THR	2.9
1	A	335	SER	2.8
1	D	418	ALA	2.8
1	E	390	SER	2.8
2	C	381	CYS	2.8
1	D	415	VAL	2.7
2	C	382	LEU	2.7
1	E	389	ALA	2.7
1	G	331	LEU	2.7
1	G	327	PHE	2.7
1	E	273	GLY	2.6
1	A	384	TYR	2.6
1	G	381	LEU	2.6
1	D	327	PHE	2.6
1	A	434	VAL	2.6
1	A	412	VAL	2.6
1	A	153	VAL	2.6
1	A	436	ILE	2.6
1	E	284	GLY	2.5
1	A	195	PHE	2.5
1	D	388	GLY	2.4
1	A	430	ASN	2.4
1	G	364	VAL	2.4
1	A	435	SER	2.4
1	A	324	GLU	2.4
1	G	208	ASP	2.3
2	F	132	ILE	2.3
1	E	354	LYS	2.3
1	G	205	SER	2.3
1	G	149	PRO	2.2
1	A	419	LEU	2.2
1	D	240	MET	2.2
1	A	163	PRO	2.2
1	G	437	MET	2.2
2	H	179	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	331	LEU	2.2
1	G	128	PHE	2.1
1	G	320	GLY	2.1
1	D	437	MET	2.1
2	B	204	ILE	2.1
1	G	413	CYS	2.1
1	G	335	SER	2.1
1	A	333	ALA	2.0
1	G	321	ARG	2.0
1	A	437	MET	2.0
1	G	251	ARG	2.0
1	A	156	ILE	2.0
1	E	420	PHE	2.0
1	G	153	VAL	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates 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.