



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:11 PM UTC

PDB ID : 5E9T / pdb_00005e9t
Title : Crystal structure of GtfA/B complex
Authors : Chen, Y.; Rapoport, T.A.
Deposited on : 2015-10-15
Resolution : 2.92 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

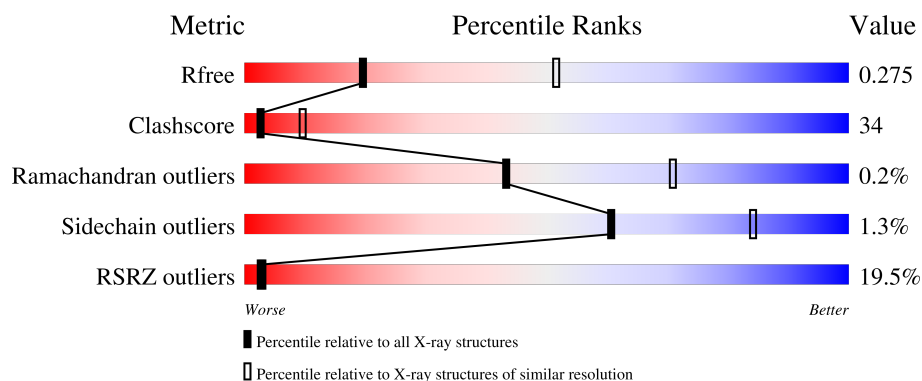
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	503	15% 61% 36% .
1	C	503	28% 54% 43% .
2	B	447	13% 54% 46% .
2	D	447	21% 49% 47% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15474 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 Glycosyltransferase Gtf1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			
1	C	503	Total	C	N	O	S	Se	0	0	0
			4108	2624	687	789	2	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q9AET5
A	124	PHE	SER	engineered mutation	UNP Q9AET5
C	1	SER	-	expression tag	UNP Q9AET5
C	124	PHE	SER	engineered mutation	UNP Q9AET5

- Molecule 2 is a protein called Glycosyltransferase-stabilizing protein Gtf2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	447	Total	C	N	O	S	Se	0	0	0
			3615	2302	615	687	3	8			
2	D	445	Total	C	N	O	S	Se	0	0	0
			3607	2298	613	685	3	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MSE	-	initiating methionine	UNP Q79T00
D	1	MSE	-	initiating methionine	UNP Q79T00

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

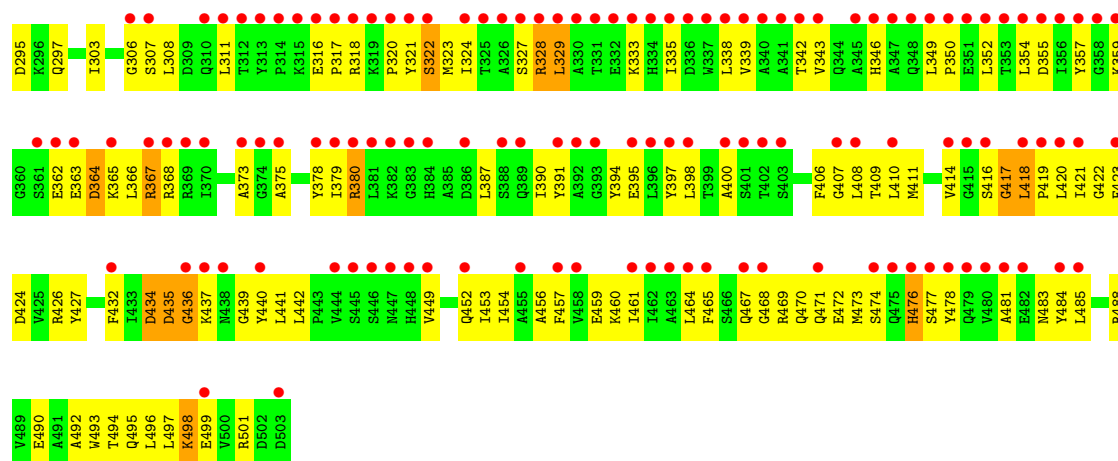
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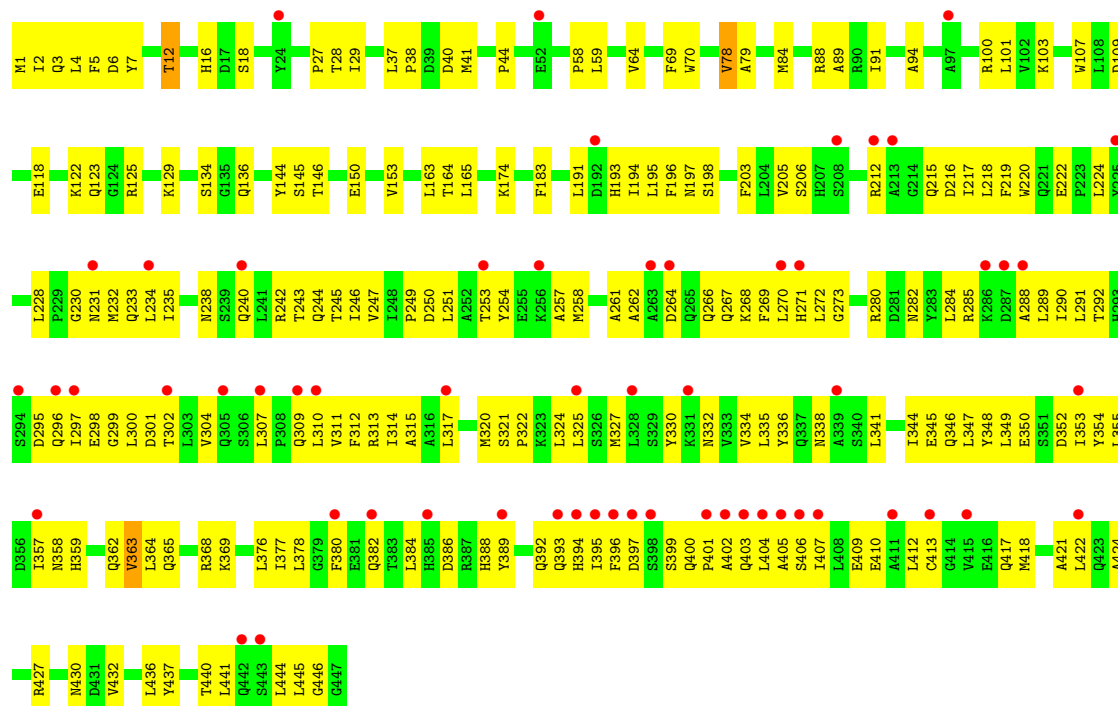
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

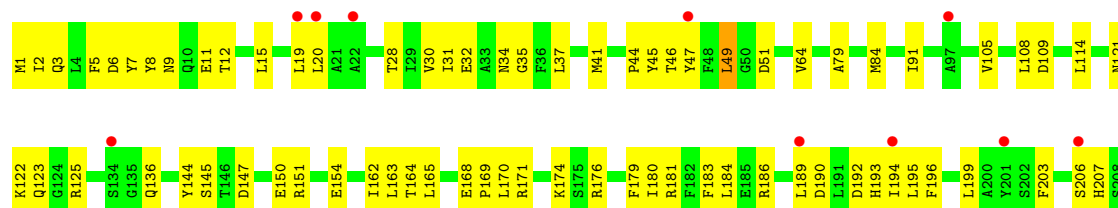
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	9	Total 9	O 9	0	0
4	C	8	Total 8	O 8	0	0
4	D	7	Total 7	O 7	0	0

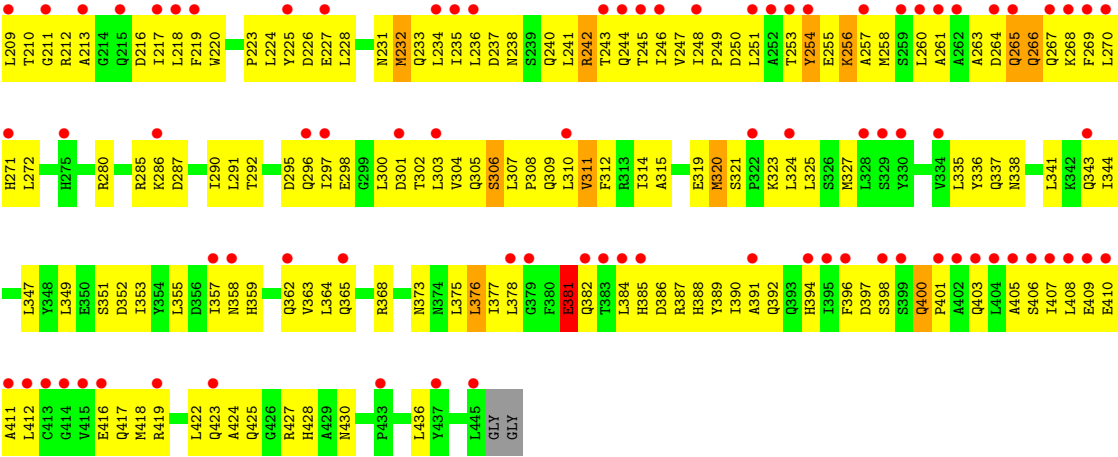


• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2



• Molecule 2: Glycosyltransferase-stabilizing protein Gtf2





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	155.93Å 196.41Å 220.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.12 – 2.92 122.12 – 2.92	Depositor EDS
% Data completeness (in resolution range)	99.9 (122.12-2.92) 99.9 (122.12-2.92)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.62Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.275 0.216 , 0.275	Depositor DCC
R_{free} test set	4641 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	15474	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.55	8/4196 (0.2%)	0.76	10/5678 (0.2%)
1	C	0.50	6/4196 (0.1%)	0.75	8/5678 (0.1%)
2	B	0.36	0/3686	0.66	0/4986
2	D	0.49	1/3678 (0.0%)	0.85	12/4976 (0.2%)
All	All	0.48	15/15756 (0.1%)	0.76	30/21318 (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	2
1	C	0	5
2	D	0	3
All	All	0	10

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	ARG	NE-CZ	-11.44	1.20	1.33
1	C	476	HIS	CE1-NE2	-9.32	1.23	1.32
1	C	418	LEU	N-CA	8.60	1.58	1.45
1	C	476	HIS	CG-ND1	-7.38	1.30	1.38
1	A	469	ARG	CZ-NH2	-6.72	1.24	1.33
1	A	469	ARG	CZ-NH1	-6.46	1.23	1.32
1	A	469	ARG	CD-NE	-6.44	1.37	1.46
1	C	476	HIS	CG-CD2	-5.97	1.29	1.35
1	C	418	LEU	C-O	5.85	1.31	1.23
1	A	472	GLU	CD-OE1	-5.81	1.14	1.25
1	A	466	SER	CA-C	5.73	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	256	LYS	CD-CE	-5.46	1.36	1.52
1	A	316	GLU	CD-OE2	-5.45	1.15	1.25
1	A	316	GLU	CD-OE1	-5.34	1.15	1.25
1	C	476	HIS	CD2-NE2	-5.17	1.32	1.37

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	ARG	NE-CZ-NH2	15.65	133.29	119.20
1	C	329	LEU	CA-CB-CG	10.42	152.78	116.30
2	D	256	LYS	CD-CE-NZ	-9.19	82.49	111.90
1	A	466	SER	N-CA-C	8.90	123.04	108.26
1	C	417	GLY	N-CA-C	8.31	126.07	114.85
1	A	488	ARG	NE-CZ-NH1	-8.21	113.29	121.50
1	A	406	PHE	CA-C-N	-8.03	105.67	121.41
1	A	406	PHE	C-N-CA	-8.03	105.67	121.41
2	D	254	TYR	CE1-CZ-OH	-7.25	98.14	119.90
2	D	254	TYR	OH-CZ-CE2	7.23	141.59	119.90
1	C	367	ARG	CD-NE-CZ	7.16	134.42	124.40
1	C	367	ARG	NE-CZ-NH1	-6.54	114.96	121.50
1	A	466	SER	CA-C-N	6.37	133.16	121.70
1	A	466	SER	C-N-CA	6.37	133.16	121.70
2	D	254	TYR	CA-CB-CG	-6.10	102.92	113.90
2	D	381	GLU	CA-C-N	-6.09	112.31	122.17
2	D	381	GLU	C-N-CA	-6.09	112.31	122.17
2	D	320	MSE	CA-C-N	6.07	128.83	120.39
2	D	320	MSE	C-N-CA	6.07	128.83	120.39
2	D	266	GLN	CA-CB-CG	-5.92	102.25	114.10
1	A	484	TYR	CD1-CE1-CZ	5.63	129.74	119.60
2	D	232	MSE	N-CA-C	-5.53	106.58	113.38
1	C	498	LYS	CD-CE-NZ	-5.44	94.49	111.90
1	C	364	ASP	N-CA-C	5.41	117.18	111.28
1	A	315	LYS	CA-C-N	5.34	134.83	121.80
1	A	315	LYS	C-N-CA	5.34	134.83	121.80
2	D	382	GLN	N-CA-C	-5.32	99.08	108.23
1	C	436	GLY	N-CA-C	-5.13	103.84	112.77
1	C	367	ARG	NH1-CZ-NH2	5.10	125.93	119.30
2	D	320	MSE	CA-CB-CG	5.07	124.24	114.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	363	GLU	Peptide
1	A	466	SER	Peptide
1	C	108	GLN	Peptide
1	C	322	SER	Peptide
1	C	328	ARG	Peptide
1	C	380	ARG	Peptide
1	C	435	ASP	Peptide
2	D	265	GLN	Peptide
2	D	381	GLU	Peptide
2	D	400	GLN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4108	0	3965	247	0
1	C	4108	0	3965	274	0
2	B	3615	0	3535	213	0
2	D	3607	0	3529	316	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	0	0	0
4	B	9	0	0	0	0
4	C	8	0	0	0	0
4	D	7	0	0	1	0
All	All	15474	0	14994	1028	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 34.

All (1028) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:307:LEU:HA	2:D:309:GLN:NE2	1.64	1.12
1:A:470:GLN:HE21	1:A:471:GLN:HG3	1.06	1.12
2:B:345:GLU:OE2	2:B:369:LYS:NZ	1.83	1.12
2:D:307:LEU:HA	2:D:309:GLN:HE21	1.13	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:272:LEU:HD13	2:B:273:GLY:H	0.92	1.07
2:D:2:ILE:HG21	2:D:189:LEU:HD12	1.36	1.07
1:A:438:ASN:HB3	1:A:476:HIS:HB3	1.35	1.06
2:B:216:ASP:HB2	2:B:243:THR:HG22	1.35	1.05
2:B:320:MSE:HB3	2:B:324:LEU:HD21	1.37	1.03
2:D:169:PRO:O	2:D:171:ARG:NH1	1.91	1.03
1:A:363:GLU:HB2	1:A:366:LEU:HB2	1.35	1.02
1:A:470:GLN:NE2	1:A:471:GLN:HG3	1.74	1.01
2:D:297:ILE:HB	2:D:300:LEU:HD23	1.37	1.00
1:C:329:LEU:HA	1:C:333:LYS:HE3	1.42	0.99
1:A:467:GLN:NE2	1:A:469:ARG:HH12	1.60	0.99
2:B:272:LEU:HD13	2:B:273:GLY:N	1.78	0.98
2:B:272:LEU:CD1	2:B:273:GLY:H	1.76	0.97
1:C:494:THR:C	1:C:498:LYS:HZ1	1.70	0.97
1:A:464:LEU:C	1:A:469:ARG:NH2	2.23	0.96
2:B:16:HIS:NE2	2:B:40:ASP:OD2	1.97	0.96
1:A:449:VAL:HG13	1:A:452:GLN:NE2	1.82	0.95
1:C:417:GLY:HA2	1:C:478:TYR:HE1	1.31	0.95
1:A:304:PRO:HG3	1:A:488:ARG:NH2	1.82	0.94
2:D:307:LEU:CA	2:D:309:GLN:HE21	1.82	0.93
1:C:12:TRP:NE1	1:C:46:ASP:OD1	2.02	0.91
1:A:464:LEU:CA	1:A:469:ARG:HH21	1.84	0.89
1:C:328:ARG:HH22	1:C:359:LYS:H	1.19	0.89
2:B:258:MSE:O	2:B:266:GLN:NE2	2.05	0.89
2:D:272:LEU:HD23	2:D:436:LEU:HD22	1.50	0.89
2:B:193:HIS:NE2	2:B:446:GLY:O	2.06	0.88
1:C:328:ARG:NH2	1:C:359:LYS:O	2.06	0.88
1:C:437:LYS:HZ3	1:C:476:HIS:CG	1.90	0.88
2:B:251:LEU:HD21	2:B:271:HIS:CE1	2.09	0.88
1:C:85:LEU:HD11	1:C:104:TYR:HE2	1.39	0.87
2:B:362:GLN:HE21	2:B:365:GLN:HA	1.38	0.87
1:C:335:ILE:HA	1:C:338:LEU:HD23	1.54	0.87
1:C:494:THR:HG22	1:C:498:LYS:NZ	1.89	0.86
1:A:369:ARG:NE	1:A:369:ARG:O	2.08	0.86
1:A:369:ARG:HH12	1:A:373:ALA:CB	1.89	0.86
2:B:1:MSE:HE3	2:B:445:LEU:HD11	1.56	0.86
2:B:270:LEU:HD21	2:B:440:THR:CG2	2.05	0.86
1:C:108:GLN:CD	1:C:109:ASP:H	1.85	0.85
2:D:220:TRP:HE1	2:D:224:LEU:HD21	1.41	0.85
1:A:369:ARG:HH12	1:A:373:ALA:HB3	1.42	0.85
2:D:11:GLU:OE2	2:D:388:HIS:HE1	1.60	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:GLY:HA2	1:C:478:TYR:CE1	2.12	0.84
2:D:125:ARG:NH2	2:D:144:TYR:O	2.10	0.84
2:D:362:GLN:HB3	2:D:384:LEU:HD21	1.59	0.84
1:A:359:LYS:NZ	1:A:384:HIS:H	1.75	0.84
2:B:376:LEU:HB2	2:B:422:LEU:HD21	1.59	0.84
1:C:397:TYR:HH	1:C:409:THR:HG1	1.15	0.83
2:B:285:ARG:NH2	2:B:349:LEU:O	2.11	0.83
1:C:335:ILE:HD11	1:C:366:LEU:HD21	1.61	0.83
1:A:449:VAL:O	1:A:452:GLN:NE2	2.12	0.83
2:D:2:ILE:HG21	2:D:189:LEU:CD1	2.09	0.83
2:D:145:SER:OG	2:D:147:ASP:OD2	1.95	0.83
2:D:220:TRP:NE1	2:D:224:LEU:HD21	1.94	0.82
1:A:462:ILE:O	1:A:466:SER:N	2.10	0.82
1:A:464:LEU:CA	1:A:469:ARG:NH2	2.42	0.82
1:A:463:ALA:C	1:A:469:ARG:HH21	1.88	0.81
1:C:349:LEU:HB3	1:C:352:LEU:HD13	1.60	0.81
1:A:382:LYS:NZ	1:A:384:HIS:O	2.12	0.81
1:C:26:GLN:HA	1:C:29:ARG:NH1	1.95	0.81
2:D:353:ILE:HG22	2:D:376:LEU:HB3	1.62	0.81
1:A:295:ASP:OD2	1:A:297:GLN:NE2	2.13	0.81
2:B:380:PHE:HD2	2:B:396:PHE:HB2	1.44	0.81
1:C:23:TYR:OH	1:C:307:SER:HB2	1.81	0.81
2:D:168:GLU:OE1	2:D:171:ARG:NH2	2.14	0.81
1:C:338:LEU:HD21	1:C:400:ALA:HB2	1.63	0.80
1:C:219:ASP:OD2	1:C:240:VAL:HG21	1.80	0.80
1:C:338:LEU:HD12	1:C:398:LEU:HB3	1.64	0.80
2:D:2:ILE:CG2	2:D:189:LEU:HD12	2.10	0.80
1:C:18:GLU:OE2	1:C:18:GLU:N	2.13	0.80
2:D:272:LEU:CD2	2:D:436:LEU:HD22	2.10	0.80
2:B:436:LEU:O	2:B:440:THR:OG1	1.99	0.79
1:A:359:LYS:HZ2	1:A:384:HIS:N	1.81	0.79
2:D:376:LEU:HG	2:D:418:MSE:HE1	1.64	0.79
1:C:435:ASP:CG	1:C:441:LEU:H	1.89	0.79
1:C:437:LYS:NZ	1:C:476:HIS:CG	2.51	0.79
1:A:334:HIS:CE1	1:A:337:TRP:CZ2	2.72	0.79
1:A:440:TYR:CD1	1:A:460:LYS:HD2	2.17	0.78
2:D:290:ILE:HD11	2:D:355:LEU:HB2	1.63	0.78
2:B:1:MSE:HE2	2:B:195:LEU:HD11	1.65	0.78
1:C:252:SER:O	1:C:293:TYR:OH	2.01	0.78
2:D:251:LEU:H	2:D:430:ASN:HD21	1.30	0.78
2:B:100:ARG:NH1	1:C:257:LEU:HD11	1.99	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ILE:HD12	1:C:454:ILE:N	1.98	0.78
2:D:184:LEU:HA	2:D:189:LEU:HD21	1.64	0.77
1:C:167:TYR:OH	2:D:150:GLU:OE2	2.01	0.77
1:A:338:LEU:HD12	1:A:338:LEU:H	1.47	0.77
1:A:30:ARG:NH1	1:A:486:THR:HG21	1.98	0.77
2:B:291:LEU:O	2:B:358:ASN:ND2	2.18	0.77
1:C:494:THR:HG22	1:C:498:LYS:HZ3	1.46	0.77
2:B:310:LEU:HB3	2:B:312:PHE:HE2	1.49	0.77
1:A:338:LEU:HD11	1:A:400:ALA:HB2	1.67	0.77
1:A:465:PHE:N	1:A:469:ARG:NH2	2.33	0.77
2:B:321:SER:O	2:B:324:LEU:HD23	1.85	0.77
2:D:307:LEU:CD1	2:D:310:LEU:HD22	2.14	0.77
2:D:381:GLU:HB3	2:D:398:SER:HB2	1.66	0.76
2:D:244:GLN:O	2:D:268:LYS:HG2	1.83	0.76
1:A:466:SER:HA	1:A:467:GLN:HE21	1.51	0.76
1:C:453:ILE:HA	1:C:456:ALA:HB3	1.68	0.76
1:C:295:ASP:O	1:C:297:GLN:NE2	2.18	0.76
2:B:288:ALA:HB3	2:B:312:PHE:HA	1.68	0.75
1:C:354:LEU:O	1:C:380:ARG:HG2	1.86	0.75
1:C:395:GLU:O	1:C:419:PRO:HD2	1.86	0.75
2:D:300:LEU:HA	2:D:303:LEU:HD23	1.68	0.75
1:A:465:PHE:C	1:A:467:GLN:HE21	1.94	0.75
1:A:30:ARG:HH12	1:A:486:THR:HG21	1.52	0.74
1:A:382:LYS:NZ	1:A:384:HIS:C	2.45	0.74
1:A:464:LEU:HA	1:A:469:ARG:HH21	1.52	0.74
2:B:270:LEU:HD23	2:B:271:HIS:N	2.02	0.74
2:D:297:ILE:CB	2:D:300:LEU:HD23	2.16	0.74
2:D:412:LEU:HD12	2:D:417:GLN:HB2	1.68	0.74
1:A:449:VAL:C	1:A:452:GLN:HE22	1.95	0.74
1:C:17:VAL:HG22	1:C:242:HIS:HD2	1.50	0.74
1:C:245:HIS:HE1	1:C:289:GLN:NE2	1.85	0.74
1:A:465:PHE:C	1:A:467:GLN:NE2	2.46	0.74
1:C:85:LEU:HD21	1:C:104:TYR:HD2	1.52	0.74
2:D:227:GLU:HA	2:D:260:LEU:HD13	1.67	0.74
2:D:397:ASP:CG	2:D:400:GLN:OE1	2.30	0.74
1:A:473:MSE:O	1:A:476:HIS:N	2.20	0.74
1:A:342:THR:HG21	1:A:354:LEU:HD23	1.70	0.74
2:D:362:GLN:HB3	2:D:384:LEU:CD2	2.18	0.73
1:C:453:ILE:HD12	1:C:454:ILE:H	1.51	0.73
1:A:304:PRO:HG3	1:A:488:ARG:HH22	1.53	0.73
2:B:285:ARG:HG2	2:B:352:ASP:OD2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:423:GLN:O	2:D:427:ARG:N	2.21	0.73
2:B:251:LEU:HD21	2:B:271:HIS:NE2	2.02	0.73
2:D:224:LEU:C	2:D:256:LYS:HZ1	1.96	0.73
1:C:328:ARG:NH2	1:C:359:LYS:H	1.84	0.73
1:A:338:LEU:HD12	1:A:338:LEU:N	2.02	0.72
1:C:181:ASP:HB2	1:C:183:GLN:HE21	1.54	0.72
2:D:263:ALA:O	2:D:266:GLN:HB2	1.88	0.72
1:A:94:ARG:HG3	1:A:105:PHE:HB2	1.72	0.72
2:B:397:ASP:HB2	2:B:401:PRO:HD3	1.69	0.72
2:D:362:GLN:NE2	2:D:365:GLN:HA	2.05	0.72
1:A:382:LYS:HD3	1:A:383:GLY:N	2.05	0.72
2:B:418:MSE:O	2:B:421:ALA:N	2.23	0.72
1:C:437:LYS:HZ3	1:C:476:HIS:C	1.97	0.71
1:C:342:THR:HG21	1:C:354:LEU:HD23	1.70	0.71
1:C:414:VAL:HG12	1:C:481:ALA:HB2	1.73	0.71
2:B:251:LEU:H	2:B:430:ASN:HD21	1.37	0.71
1:C:496:LEU:HD12	1:C:499:GLU:OE1	1.89	0.71
2:D:412:LEU:HD12	2:D:417:GLN:CB	2.20	0.71
2:D:397:ASP:OD2	2:D:400:GLN:OE1	2.08	0.71
1:A:461:ILE:O	1:A:465:PHE:N	2.23	0.71
2:B:270:LEU:HD21	2:B:440:THR:HG21	1.71	0.70
1:C:498:LYS:H	1:C:498:LYS:HD2	1.56	0.70
2:B:362:GLN:NE2	2:B:365:GLN:HA	2.06	0.70
1:C:335:ILE:HD11	1:C:366:LEU:CD2	2.20	0.70
1:C:421:ILE:HD12	1:C:440:TYR:HB2	1.74	0.70
1:A:465:PHE:N	1:A:469:ARG:HH22	1.86	0.70
1:C:453:ILE:O	1:C:457:PHE:N	2.24	0.70
2:D:168:GLU:HB3	2:D:171:ARG:HH12	1.55	0.70
1:C:329:LEU:HD11	1:C:363:GLU:HB2	1.72	0.70
1:C:338:LEU:HD12	1:C:398:LEU:HD13	1.73	0.69
2:D:189:LEU:HD23	2:D:189:LEU:H	1.57	0.69
1:A:387:LEU:HA	1:A:390:ILE:HD13	1.75	0.69
1:A:470:GLN:HE21	1:A:471:GLN:CG	1.95	0.69
2:B:100:ARG:HH11	1:C:257:LEU:HD11	1.57	0.69
2:B:359:HIS:HD2	2:B:382:GLN:HE21	1.40	0.69
2:D:401:PRO:HB2	2:D:403:GLN:OE1	1.91	0.69
2:D:384:LEU:C	2:D:384:LEU:HD23	2.18	0.69
2:B:376:LEU:HD11	2:B:394:HIS:CD2	2.28	0.69
1:C:397:TYR:HB3	1:C:420:LEU:CD1	2.23	0.69
2:B:4:LEU:CD2	2:B:205:VAL:HG21	2.23	0.69
1:C:321:TYR:N	1:C:395:GLU:OE1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:295:ASP:OD1	2:D:321:SER:OG	2.11	0.69
2:D:37:LEU:O	2:D:122:LYS:NZ	2.24	0.68
1:C:437:LYS:NZ	1:C:476:HIS:CD2	2.61	0.68
2:D:287:ASP:HB2	2:D:351:SER:HA	1.76	0.68
2:D:417:GLN:H	2:D:417:GLN:CD	2.00	0.68
1:A:464:LEU:HA	1:A:469:ARG:NH2	2.06	0.68
1:A:464:LEU:HD13	1:A:473:MSE:HE3	1.75	0.68
2:D:218:LEU:HD11	2:D:220:TRP:HB2	1.75	0.68
1:C:363:GLU:HG3	1:C:367:ARG:HE	1.58	0.68
2:D:286:LYS:HD2	2:D:310:LEU:HA	1.75	0.68
2:B:79:ALA:HB3	2:B:91:ILE:HB	1.74	0.68
2:B:405:ALA:O	2:B:409:GLU:N	2.18	0.68
1:C:492:ALA:HA	1:C:495:GLN:HB3	1.76	0.68
2:B:362:GLN:HA	2:B:384:LEU:HD23	1.74	0.68
2:D:412:LEU:CD1	2:D:417:GLN:HB2	2.24	0.68
1:A:485:LEU:O	1:A:488:ARG:HG3	1.94	0.68
2:D:292:THR:HA	2:D:358:ASN:HD22	1.57	0.68
2:B:320:MSE:CB	2:B:324:LEU:HD21	2.20	0.67
2:D:307:LEU:HD13	2:D:310:LEU:HD22	1.74	0.67
2:D:295:ASP:OD2	2:D:323:LYS:HG2	1.92	0.67
2:B:338:ASN:O	1:C:249:ASN:ND2	2.24	0.67
2:B:399:SER:HA	2:B:402:ALA:HA	1.75	0.67
1:C:434:ASP:OD1	1:C:434:ASP:N	2.27	0.67
2:D:184:LEU:HD22	2:D:189:LEU:HD11	1.75	0.67
2:D:255:GLU:N	2:D:255:GLU:OE1	2.28	0.67
2:D:397:ASP:OD2	2:D:400:GLN:CD	2.37	0.67
1:C:323:MSE:HB3	1:C:354:LEU:HA	1.75	0.67
2:B:322:PRO:HA	2:B:325:LEU:HB2	1.75	0.67
1:C:323:MSE:HB3	1:C:354:LEU:CA	2.25	0.67
2:D:45:TYR:O	2:D:49:LEU:HD11	1.95	0.67
1:C:180:GLU:O	1:C:183:GLN:HG3	1.95	0.66
2:D:419:ARG:C	2:D:423:GLN:HE22	2.01	0.66
2:B:407:ILE:HA	2:B:410:GLU:HB2	1.77	0.66
1:C:364:ASP:O	1:C:368:ARG:HG3	1.95	0.66
2:D:233:GLN:HA	2:D:236:LEU:HG	1.77	0.66
2:D:417:GLN:N	2:D:417:GLN:OE1	2.27	0.66
1:A:382:LYS:HZ3	1:A:383:GLY:C	2.03	0.66
2:B:359:HIS:HD2	2:B:382:GLN:NE2	1.94	0.66
2:D:224:LEU:HB3	2:D:256:LYS:CE	2.25	0.66
2:D:236:LEU:O	2:D:268:LYS:NZ	2.23	0.66
2:D:254:TYR:O	2:D:257:ALA:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:VAL:HG12	1:C:276:ILE:HB	1.78	0.66
1:C:362:GLU:O	1:C:366:LEU:HD12	1.96	0.66
1:C:3:VAL:HG22	1:C:215:VAL:HB	1.78	0.66
2:D:220:TRP:HE1	2:D:224:LEU:CD2	2.07	0.66
2:B:125:ARG:NH1	2:B:146:THR:HA	2.11	0.66
2:B:272:LEU:HD11	2:B:437:TYR:CE1	2.30	0.66
2:D:219:PHE:CD1	2:D:247:VAL:CG1	2.79	0.66
2:D:295:ASP:HB2	2:D:296:GLN:HA	1.78	0.66
2:D:381:GLU:OE2	2:D:387:ARG:NH2	2.28	0.66
1:C:85:LEU:HD11	1:C:104:TYR:CE2	2.28	0.66
2:D:227:GLU:OE2	2:D:228:LEU:N	2.27	0.66
2:D:224:LEU:HB3	2:D:256:LYS:HE2	1.77	0.66
2:D:418:MSE:HG3	2:D:422:LEU:HD11	1.78	0.66
2:B:1:MSE:HE3	2:B:445:LEU:CD1	2.26	0.65
1:C:27:ILE:HG23	1:C:490:GLU:HG2	1.77	0.65
1:C:85:LEU:HD21	1:C:104:TYR:CD2	2.30	0.65
1:A:363:GLU:HB2	1:A:366:LEU:CB	2.20	0.65
1:A:321:TYR:CD2	1:A:349:LEU:HD11	2.32	0.65
2:B:282:ASN:HD21	2:B:418:MSE:HE3	1.62	0.65
2:D:412:LEU:HA	2:D:417:GLN:HG3	1.78	0.65
1:A:315:LYS:C	1:A:317:PRO:HD3	2.21	0.65
2:D:219:PHE:CD1	2:D:247:VAL:HG11	2.30	0.65
2:D:220:TRP:CE2	2:D:224:LEU:HD21	2.32	0.65
1:A:3:VAL:HG22	1:A:215:VAL:HB	1.79	0.65
1:C:244:GLU:OE2	1:C:427:TYR:OH	2.08	0.65
1:C:329:LEU:CA	1:C:333:LYS:HE3	2.25	0.65
1:C:440:TYR:CD1	1:C:460:LYS:HD2	2.32	0.65
2:D:190:ASP:OD1	2:D:192:ASP:OD2	2.14	0.65
1:C:23:TYR:CE2	1:C:27:ILE:HD11	2.32	0.65
2:D:218:LEU:CD1	2:D:220:TRP:HB2	2.26	0.65
2:D:307:LEU:C	2:D:309:GLN:HE21	2.05	0.65
2:B:264:ASP:O	2:B:267:GLN:NE2	2.30	0.64
2:D:286:LYS:NZ	2:D:310:LEU:CD1	2.60	0.64
2:B:270:LEU:HD21	2:B:440:THR:HG22	1.80	0.64
2:D:238:ASN:ND2	2:D:241:LEU:HB2	2.12	0.64
1:C:434:ASP:HB2	1:C:437:LYS:HB3	1.78	0.64
2:B:4:LEU:HD12	2:B:29:ILE:HB	1.79	0.64
2:B:125:ARG:HH11	2:B:146:THR:HA	1.62	0.64
2:B:393:GLN:OE1	2:B:424:ALA:HB1	1.98	0.64
1:C:435:ASP:OD1	1:C:441:LEU:N	2.31	0.64
2:D:216:ASP:OD1	2:D:242:ARG:HG3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:MSE:SE	2:D:324:LEU:HD22	2.48	0.64
1:A:259:ASN:HD22	1:A:260:ASN:N	1.95	0.63
1:C:342:THR:HG21	1:C:354:LEU:CD2	2.29	0.63
1:A:440:TYR:CZ	1:A:473:MSE:HE1	2.33	0.63
2:B:194:ILE:O	2:B:216:ASP:HB3	1.98	0.63
2:D:286:LYS:NZ	2:D:310:LEU:HD12	2.13	0.63
2:D:287:ASP:HA	2:D:311:VAL:HG13	1.80	0.63
1:C:7:ASN:OD1	1:C:8:LEU:N	2.30	0.63
1:C:199:GLU:OE2	1:C:202:ARG:NH1	2.32	0.63
2:D:298:GLU:OE2	2:D:359:HIS:NE2	2.24	0.63
1:A:11:GLY:H	1:A:14:SER:HB2	1.64	0.63
1:C:495:GLN:HA	1:C:498:LYS:HZ2	1.64	0.63
2:B:251:LEU:CD2	2:B:271:HIS:CE1	2.82	0.62
2:D:412:LEU:HD12	2:D:417:GLN:C	2.24	0.62
1:C:459:GLU:OE1	1:C:460:LYS:HG2	2.00	0.62
2:D:194:ILE:O	2:D:216:ASP:HB2	2.00	0.62
2:B:313:ARG:HA	2:B:334:VAL:O	1.99	0.62
1:C:397:TYR:HD1	1:C:420:LEU:HD11	1.65	0.62
1:A:469:ARG:HA	1:A:472:GLU:HB3	1.82	0.62
2:D:254:TYR:CZ	2:D:258:MSE:HG3	2.34	0.62
2:D:409:GLU:HA	2:D:412:LEU:HD22	1.81	0.62
1:C:440:TYR:CD2	1:C:460:LYS:HB3	2.35	0.62
2:B:377:ILE:O	2:B:378:LEU:HD23	2.00	0.62
1:A:397:TYR:HB3	1:A:420:LEU:CD1	2.30	0.62
1:A:449:VAL:HG13	1:A:452:GLN:HE22	1.65	0.61
2:B:314:ILE:HB	2:B:335:LEU:HD22	1.81	0.61
2:D:307:LEU:HD11	2:D:406:SER:HB2	1.82	0.61
2:B:250:ASP:HA	2:B:430:ASN:ND2	2.15	0.61
1:C:17:VAL:HG22	1:C:242:HIS:CD2	2.35	0.61
1:C:110:ASP:OD1	1:C:110:ASP:N	2.21	0.61
1:C:363:GLU:O	1:C:367:ARG:HG2	2.00	0.61
2:D:79:ALA:HB3	2:D:91:ILE:HB	1.80	0.61
2:D:286:LYS:CE	2:D:310:LEU:HD12	2.31	0.61
1:A:119:GLN:HB2	1:A:122:GLN:HG3	1.82	0.61
1:A:414:VAL:HG23	1:A:420:LEU:HD21	1.83	0.61
2:B:272:LEU:HD11	2:B:437:TYR:CZ	2.35	0.61
1:C:395:GLU:O	1:C:419:PRO:CD	2.48	0.61
1:C:476:HIS:ND1	1:C:476:HIS:O	2.34	0.61
2:B:6:ASP:OD2	2:B:198:SER:HB3	2.01	0.61
1:C:245:HIS:HB2	1:C:266:PHE:HE2	1.66	0.61
2:D:261:ALA:HB1	2:D:265:GLN:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLU:O	1:A:419:PRO:HD2	2.01	0.61
2:B:282:ASN:OD1	2:B:284:LEU:N	2.25	0.61
2:B:400:GLN:HB2	2:B:401:PRO:HD3	1.83	0.61
2:B:427:ARG:HG2	2:B:427:ARG:HH11	1.66	0.61
2:D:397:ASP:OD1	2:D:401:PRO:HD2	2.01	0.61
1:A:15:SER:HA	1:A:19:TYR:HD2	1.66	0.60
1:A:370:ILE:HG22	1:A:371:GLU:CD	2.26	0.60
2:B:203:PHE:HE2	2:B:231:ASN:OD1	1.84	0.60
2:D:300:LEU:O	2:D:304:VAL:HG23	2.01	0.60
1:C:323:MSE:HE2	1:C:342:THR:HG22	1.84	0.60
2:D:246:ILE:HB	2:D:269:PHE:HB3	1.83	0.60
1:A:476:HIS:O	1:A:480:VAL:HG22	2.02	0.60
1:A:483:ASN:O	1:A:488:ARG:HD3	2.00	0.60
2:D:305:GLN:HG2	2:D:306:SER:N	2.16	0.60
1:C:437:LYS:NZ	1:C:476:HIS:C	2.59	0.60
2:D:7:TYR:O	2:D:12:THR:HG21	2.01	0.60
2:D:416:GLU:N	2:D:417:GLN:OE1	2.35	0.60
2:B:378:LEU:HD21	2:B:394:HIS:HD2	1.67	0.60
1:C:165:ARG:HG3	1:C:176:ASP:HB3	1.84	0.60
2:B:230:GLY:O	2:B:233:GLN:HB2	2.01	0.60
2:B:307:LEU:HD11	2:B:406:SER:HB2	1.83	0.59
2:B:332:ASN:O	2:B:332:ASN:ND2	2.35	0.59
1:C:245:HIS:HE1	1:C:289:GLN:HE22	1.47	0.59
1:C:343:VAL:HG21	1:C:373:ALA:HB1	1.83	0.59
2:D:195:LEU:HA	2:D:217:ILE:HD11	1.85	0.59
2:D:217:ILE:HD12	2:D:217:ILE:C	2.27	0.59
1:A:345:ALA:HB2	1:A:458:VAL:HG23	1.85	0.59
2:D:396:PHE:CD2	2:D:405:ALA:HA	2.36	0.59
1:A:440:TYR:HD1	1:A:460:LYS:HB3	1.66	0.59
1:A:467:GLN:HA	1:A:469:ARG:NH1	2.18	0.59
2:D:234:LEU:HD12	2:D:235:ILE:HB	1.85	0.59
1:A:318:ARG:NH1	1:A:394:TYR:O	2.35	0.59
2:B:4:LEU:HD21	2:B:205:VAL:HG21	1.85	0.59
2:B:125:ARG:HH12	2:B:145:SER:C	2.10	0.59
1:C:117:LEU:HD21	1:C:122:GLN:O	2.02	0.59
1:C:424:ASP:HB2	1:C:441:LEU:HB3	1.84	0.59
2:D:392:GLN:C	2:D:394:HIS:H	2.09	0.59
2:B:301:ASP:N	2:B:327:MSE:HE1	2.17	0.58
1:C:211:GLN:HG2	1:C:212:ALA:H	1.68	0.58
1:C:363:GLU:HA	1:C:366:LEU:HD13	1.84	0.58
2:D:234:LEU:HD12	2:D:235:ILE:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:GLN:N	1:A:310:GLN:OE1	2.36	0.58
1:A:464:LEU:N	1:A:469:ARG:HH21	1.99	0.58
1:C:47:ASN:HB3	1:C:50:HIS:CE1	2.39	0.58
2:D:227:GLU:CD	2:D:228:LEU:H	2.12	0.58
2:D:249:PRO:O	2:D:430:ASN:ND2	2.35	0.58
1:C:27:ILE:HD12	1:C:27:ILE:H	1.68	0.58
1:C:101:ILE:O	1:C:101:ILE:HG13	2.02	0.58
2:D:319:GLU:HG2	2:D:338:ASN:HD21	1.69	0.58
2:D:227:GLU:CD	2:D:228:LEU:N	2.61	0.58
1:A:189:PHE:HB2	1:A:192:ARG:HB2	1.85	0.58
1:A:323:MSE:HE3	1:A:352:LEU:HD11	1.86	0.58
2:B:341:LEU:O	2:B:344:ILE:HG22	2.04	0.58
1:A:337:TRP:CH2	1:A:453:ILE:HD13	2.39	0.58
1:A:363:GLU:CB	1:A:366:LEU:HB2	2.24	0.58
1:C:88:VAL:HG21	1:C:113:ILE:HD13	1.84	0.58
2:D:220:TRP:CZ2	2:D:224:LEU:HD21	2.38	0.58
1:A:440:TYR:CE1	1:A:460:LYS:HD2	2.38	0.58
2:B:249:PRO:HA	2:B:272:LEU:O	2.03	0.58
1:C:422:GLY:O	1:C:441:LEU:HA	2.04	0.58
1:C:494:THR:HG22	1:C:498:LYS:HZ1	1.68	0.58
2:D:224:LEU:HB2	2:D:256:LYS:HZ3	1.68	0.58
2:D:324:LEU:O	2:D:327:MSE:HG2	2.04	0.58
2:D:336:TYR:CD1	2:D:347:LEU:HD21	2.38	0.58
2:D:343:GLN:O	2:D:347:LEU:HD12	2.03	0.58
2:D:231:ASN:O	2:D:234:LEU:HG	2.03	0.58
1:C:354:LEU:HG	1:C:379:ILE:HG12	1.85	0.58
2:D:300:LEU:CD1	2:D:327:MSE:HE2	2.34	0.58
2:D:397:ASP:OD2	2:D:400:GLN:NE2	2.36	0.58
1:A:437:LYS:HB3	1:A:476:HIS:CD2	2.39	0.57
1:A:81:LEU:HD21	1:A:102:VAL:HG21	1.85	0.57
1:A:465:PHE:CA	1:A:469:ARG:HH22	2.16	0.57
1:C:437:LYS:HD3	1:C:476:HIS:CD2	2.39	0.57
2:B:401:PRO:HB2	2:B:404:LEU:HB2	1.85	0.57
2:D:386:ASP:HB3	2:D:388:HIS:HB2	1.86	0.57
1:A:7:ASN:OD1	1:A:8:LEU:N	2.36	0.57
1:C:111:GLN:OE1	2:D:174:LYS:NZ	2.36	0.57
1:C:161:LEU:HD21	1:C:164:ARG:HH12	1.69	0.57
2:D:296:GLN:HB2	2:D:323:LYS:HE2	1.85	0.57
1:A:363:GLU:CD	1:A:363:GLU:N	2.63	0.57
2:D:290:ILE:CD1	2:D:355:LEU:HB2	2.33	0.57
1:C:437:LYS:HZ2	1:C:476:HIS:CD2	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:GLU:CD	1:C:460:LYS:N	2.63	0.57
2:B:203:PHE:HE2	2:B:231:ASN:CG	2.13	0.57
1:A:367:ARG:HB3	1:A:368:ARG:NH1	2.20	0.57
1:A:482:GLU:HA	1:A:485:LEU:HD13	1.86	0.57
1:A:488:ARG:CZ	1:A:489:VAL:HG22	2.35	0.57
1:C:474:SER:O	1:C:477:SER:HB3	2.05	0.57
2:B:58:PRO:HB2	2:B:101:LEU:HD12	1.86	0.57
2:B:386:ASP:HB3	2:B:388:HIS:ND1	2.20	0.57
1:C:27:ILE:HG22	1:C:31:ILE:HD11	1.87	0.57
1:C:397:TYR:HB3	1:C:420:LEU:HD13	1.87	0.57
2:D:423:GLN:H	2:D:423:GLN:CD	2.13	0.57
1:A:476:HIS:HA	1:A:479:GLN:HB2	1.86	0.56
1:A:483:ASN:O	1:A:488:ARG:NH1	2.38	0.56
1:C:24:ARG:HH12	1:C:219:ASP:CG	2.12	0.56
1:C:420:LEU:O	1:C:439:GLY:HA3	2.05	0.56
1:C:432:PHE:HE1	1:C:484:TYR:CD2	2.24	0.56
2:D:363:VAL:HG12	2:D:364:LEU:HG	1.87	0.56
1:A:466:SER:N	1:A:469:ARG:HH22	2.02	0.56
2:B:193:HIS:ND1	2:B:215:GLN:O	2.37	0.56
2:B:380:PHE:CD2	2:B:396:PHE:HB2	2.34	0.56
1:C:321:TYR:H	1:C:395:GLU:CD	2.12	0.56
2:D:181:ARG:HE	2:D:209:LEU:HD21	1.69	0.56
1:A:369:ARG:HH12	1:A:373:ALA:HB2	1.68	0.56
1:C:316:GLU:HB3	1:C:317:PRO:HD2	1.87	0.56
2:B:232:MSE:HE3	2:B:246:ILE:HG21	1.87	0.56
2:D:320:MSE:HE3	2:D:335:LEU:HD13	1.87	0.56
2:B:282:ASN:ND2	2:B:418:MSE:HE3	2.20	0.56
2:B:410:GLU:C	2:B:412:LEU:H	2.13	0.56
1:C:323:MSE:HE3	1:C:398:LEU:HD11	1.87	0.56
1:A:417:GLY:HA2	1:A:477:SER:HB2	1.87	0.56
1:C:202:ARG:NH2	1:C:230:GLU:OE1	2.39	0.56
2:D:195:LEU:HA	2:D:217:ILE:CD1	2.36	0.56
2:D:207:HIS:CD2	2:D:241:LEU:HD11	2.41	0.56
2:D:235:ILE:HD11	2:D:243:THR:O	2.05	0.56
2:D:254:TYR:CZ	2:D:271:HIS:NE2	2.74	0.56
1:A:80:THR:OG1	1:A:83:GLN:HG3	2.06	0.56
1:A:284:ARG:O	1:A:288:GLN:NE2	2.39	0.56
2:B:267:GLN:OE1	2:B:267:GLN:N	2.36	0.56
1:C:221:GLU:HG2	1:C:225:GLY:HA3	1.87	0.56
2:D:168:GLU:HB3	2:D:171:ARG:HH22	1.71	0.56
1:A:341:ALA:HA	1:A:454:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:HD13	1:A:370:ILE:CD1	2.36	0.55
2:D:240:GLN:HA	2:D:240:GLN:OE1	2.07	0.55
1:A:349:LEU:HD22	1:A:350:PRO:HD2	1.88	0.55
1:C:113:ILE:HG13	1:C:113:ILE:O	2.07	0.55
1:C:494:THR:CG2	1:C:498:LYS:NZ	2.66	0.55
1:A:438:ASN:CB	1:A:476:HIS:HB3	2.24	0.55
2:B:164:THR:HG23	2:B:164:THR:O	2.06	0.55
1:C:335:ILE:O	1:C:339:VAL:N	2.37	0.55
1:A:327:SER:O	1:A:358:GLY:HA3	2.06	0.55
2:B:413:CYS:SG	2:B:417:GLN:NE2	2.80	0.55
1:C:338:LEU:CD1	1:C:398:LEU:HB3	2.35	0.55
2:D:196:PHE:CE2	2:D:218:LEU:HD23	2.41	0.55
2:B:270:LEU:HD11	2:B:440:THR:HG22	1.88	0.55
2:B:309:GLN:OE1	2:B:309:GLN:N	2.23	0.55
1:C:395:GLU:HG2	1:C:470:GLN:NE2	2.22	0.55
2:D:32:GLU:OE2	2:D:34:ASN:HB2	2.07	0.55
2:D:291:LEU:HD13	2:D:344:ILE:HD11	1.87	0.55
2:B:258:MSE:SE	2:B:266:GLN:HB3	2.55	0.55
1:A:366:LEU:CD1	1:A:370:ILE:HD11	2.36	0.55
1:C:24:ARG:NH1	1:C:219:ASP:OD1	2.40	0.55
2:B:297:ILE:H	2:B:297:ILE:HD12	1.71	0.55
1:C:173:VAL:HG21	2:D:144:TYR:HE2	1.71	0.55
2:D:190:ASP:OD1	2:D:192:ASP:CG	2.50	0.55
2:D:287:ASP:OD1	2:D:311:VAL:HG11	2.07	0.55
2:B:272:LEU:CD1	2:B:273:GLY:O	2.56	0.54
1:C:321:TYR:N	1:C:395:GLU:CD	2.65	0.54
2:D:280:ARG:NH2	2:D:352:ASP:OD1	2.39	0.54
1:A:44:LEU:HB3	1:A:141:TYR:CE2	2.42	0.54
2:B:295:ASP:CB	2:B:296:GLN:HA	2.31	0.54
1:A:278:ALA:HB1	1:A:406:PHE:HB2	1.90	0.54
1:A:471:GLN:O	1:A:475:GLN:HG3	2.07	0.54
2:D:168:GLU:CB	2:D:171:ARG:HH12	2.18	0.54
2:D:362:GLN:HE22	2:D:365:GLN:HA	1.70	0.54
1:C:432:PHE:HE1	1:C:484:TYR:CE2	2.26	0.54
2:D:228:LEU:HD22	2:D:232:MSE:SE	2.57	0.54
1:A:359:LYS:HB2	1:A:384:HIS:NE2	2.23	0.54
1:C:355:ASP:OD2	1:C:380:ARG:HG3	2.07	0.54
2:D:250:ASP:OD2	2:D:253:THR:OG1	2.24	0.54
1:A:363:GLU:CD	1:A:363:GLU:H	2.16	0.54
2:D:258:MSE:SE	2:D:266:GLN:OE1	2.76	0.54
2:D:320:MSE:HG2	2:D:337:GLN:CD	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:MSE:HE2	1:C:199:GLU:OE2	2.07	0.54
2:D:408:LEU:O	2:D:411:ALA:HB3	2.08	0.54
1:A:414:VAL:HG12	1:A:481:ALA:HB2	1.88	0.54
1:A:449:VAL:HG13	1:A:452:GLN:CD	2.31	0.54
2:B:362:GLN:CA	2:B:384:LEU:HD23	2.38	0.54
1:A:337:TRP:O	1:A:341:ALA:N	2.41	0.54
2:B:295:ASP:HB2	2:B:296:GLN:HA	1.90	0.54
1:C:437:LYS:HD3	1:C:476:HIS:NE2	2.23	0.54
1:C:449:VAL:O	1:C:452:GLN:HB2	2.08	0.54
2:D:287:ASP:HA	2:D:311:VAL:CG1	2.38	0.54
1:C:424:ASP:HA	1:C:441:LEU:HD22	1.91	0.53
1:C:456:ALA:O	1:C:459:GLU:OE1	2.26	0.53
2:D:3:GLN:NE2	2:D:19:LEU:HD21	2.22	0.53
2:D:176:ARG:O	2:D:180:ILE:HG13	2.09	0.53
2:D:368:ARG:HB2	2:D:389:TYR:HE2	1.73	0.53
1:A:359:LYS:NZ	1:A:383:GLY:HA3	2.23	0.53
2:D:307:LEU:HD11	2:D:406:SER:CB	2.38	0.53
1:A:495:GLN:NE2	1:A:499:GLU:OE2	2.40	0.53
2:B:290:ILE:HG13	2:B:357:ILE:HD11	1.90	0.53
2:D:391:ALA:O	2:D:394:HIS:HB2	2.07	0.53
1:A:359:LYS:HG3	1:A:384:HIS:CG	2.44	0.53
2:D:321:SER:C	2:D:325:LEU:HD12	2.32	0.53
2:B:69:PHE:CZ	1:C:271:LYS:HD2	2.43	0.53
2:B:125:ARG:NH1	2:B:145:SER:O	2.42	0.53
2:D:307:LEU:HD12	2:D:310:LEU:HD22	1.89	0.53
1:A:143:SER:OG	1:A:144:TYR:N	2.37	0.53
1:A:396:LEU:HD12	1:A:419:PRO:O	2.08	0.53
2:D:163:LEU:HD13	2:D:179:PHE:HE1	1.73	0.53
2:D:290:ILE:HD13	2:D:355:LEU:O	2.08	0.53
2:D:300:LEU:HD11	2:D:327:MSE:HE2	1.90	0.53
2:D:310:LEU:HD23	2:D:312:PHE:CZ	2.44	0.53
1:C:81:LEU:H	1:C:81:LEU:HD12	1.73	0.53
1:C:108:GLN:CD	1:C:109:ASP:N	2.63	0.53
1:C:195:TYR:CE1	2:D:109:ASP:HA	2.44	0.53
2:B:196:PHE:CE2	2:B:218:LEU:HB2	2.44	0.53
1:C:338:LEU:CD2	1:C:400:ALA:HB2	2.38	0.53
1:C:378:TYR:O	1:C:379:ILE:HG13	2.09	0.53
2:D:297:ILE:HG22	2:D:357:ILE:HG22	1.91	0.53
2:D:1:MSE:N	2:D:190:ASP:O	2.30	0.53
2:D:258:MSE:SE	2:D:266:GLN:CD	3.02	0.53
1:A:244:GLU:OE2	1:A:427:TYR:CE1	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ILE:C	1:A:465:PHE:H	2.16	0.52
2:B:18:SER:HB3	2:B:437:TYR:CZ	2.44	0.52
2:B:297:ILE:HG21	2:B:357:ILE:HD12	1.91	0.52
2:D:219:PHE:HD1	2:D:247:VAL:HG11	1.74	0.52
2:D:424:ALA:HA	2:D:427:ARG:HG2	1.89	0.52
1:A:173:VAL:HG21	2:B:144:TYR:HE2	1.74	0.52
1:A:339:VAL:O	1:A:343:VAL:HG13	2.09	0.52
1:C:26:GLN:HA	1:C:29:ARG:HH12	1.74	0.52
2:D:286:LYS:CD	2:D:310:LEU:HD12	2.39	0.52
2:B:315:ALA:HA	2:B:336:TYR:O	2.09	0.52
1:C:329:LEU:HA	1:C:333:LYS:CE	2.27	0.52
2:D:368:ARG:HD3	2:D:389:TYR:CE2	2.45	0.52
2:B:403:GLN:HE21	2:B:404:LEU:HD12	1.74	0.52
1:A:15:SER:HA	1:A:19:TYR:CD2	2.44	0.52
1:A:438:ASN:HA	1:A:473:MSE:HB3	1.91	0.52
1:A:467:GLN:HE22	1:A:469:ARG:HH12	1.49	0.52
1:C:495:GLN:HA	1:C:498:LYS:NZ	2.24	0.52
1:C:245:HIS:HB2	1:C:266:PHE:CE2	2.43	0.52
2:D:286:LYS:NZ	2:D:310:LEU:HD11	2.25	0.52
1:C:327:SER:O	1:C:333:LYS:NZ	2.41	0.52
2:D:306:SER:O	2:D:307:LEU:HD23	2.10	0.52
1:A:42:MSE:HE3	1:A:164:ARG:HH11	1.75	0.51
2:B:396:PHE:CZ	2:B:405:ALA:HA	2.45	0.51
2:D:11:GLU:OE2	2:D:388:HIS:CE1	2.52	0.51
1:A:144:TYR:CD1	1:A:145:VAL:HG23	2.45	0.51
1:A:359:LYS:HZ1	1:A:383:GLY:HA3	1.75	0.51
2:B:271:HIS:CE1	2:B:272:LEU:O	2.64	0.51
2:B:320:MSE:SE	2:B:324:LEU:HD11	2.59	0.51
2:B:407:ILE:HA	2:B:410:GLU:CB	2.40	0.51
2:B:441:LEU:O	2:B:444:LEU:N	2.37	0.51
1:A:241:VAL:HA	1:A:262:TYR:CE1	2.45	0.51
1:A:270:ASP:OD2	1:A:271:LYS:HE3	2.10	0.51
1:A:369:ARG:O	1:A:369:ARG:CZ	2.58	0.51
1:A:382:LYS:HD3	1:A:382:LYS:C	2.35	0.51
1:C:437:LYS:O	1:C:473:MSE:SE	2.79	0.51
2:D:212:ARG:HG3	2:D:213:ALA:N	2.25	0.51
2:D:236:LEU:HD12	2:D:237:ASP:N	2.25	0.51
2:B:282:ASN:HD22	2:B:422:LEU:HD11	1.76	0.51
1:C:397:TYR:HB3	1:C:420:LEU:HD11	1.91	0.51
1:C:406:PHE:CZ	1:C:411:MSE:HE2	2.45	0.51
2:D:5:PHE:O	2:D:30:VAL:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:LEU:N	2:D:165:LEU:HD22	2.25	0.51
2:D:181:ARG:HH11	2:D:209:LEU:CD1	2.23	0.51
1:A:420:LEU:HB2	1:A:433:ILE:HG12	1.92	0.51
2:D:6:ASP:HA	2:D:31:ILE:HG13	1.93	0.51
2:B:280:ARG:HH21	2:B:349:LEU:HA	1.76	0.51
2:B:368:ARG:NH1	2:B:389:TYR:OH	2.40	0.51
1:C:17:VAL:HG13	1:C:242:HIS:CD2	2.46	0.51
1:C:31:ILE:HG12	1:C:494:THR:OG1	2.11	0.51
1:C:81:LEU:O	1:C:85:LEU:HD12	2.10	0.51
2:D:254:TYR:CE2	2:D:258:MSE:HG3	2.46	0.51
2:B:247:VAL:HG12	2:B:249:PRO:HD3	1.93	0.51
2:D:196:PHE:HE2	2:D:218:LEU:HD23	1.75	0.51
1:A:404:GLU:O	1:A:427:TYR:N	2.34	0.51
2:B:289:LEU:HD13	2:B:347:LEU:HB3	1.93	0.51
1:C:323:MSE:HB3	1:C:354:LEU:HB3	1.92	0.51
2:D:254:TYR:CZ	2:D:258:MSE:HE3	2.45	0.51
2:D:307:LEU:HB3	2:D:310:LEU:HB2	1.93	0.51
1:A:85:LEU:HD11	1:A:104:TYR:CZ	2.46	0.51
2:D:409:GLU:HA	2:D:412:LEU:CD2	2.41	0.51
1:A:244:GLU:OE2	1:A:427:TYR:HE1	1.94	0.51
2:B:37:LEU:O	2:B:122:LYS:NZ	2.39	0.51
1:C:117:LEU:HD11	1:C:123:ASP:C	2.36	0.51
2:D:267:GLN:CD	2:D:267:GLN:H	2.19	0.51
2:D:391:ALA:HB3	2:D:394:HIS:HD2	1.76	0.51
2:B:264:ASP:OD1	2:B:264:ASP:N	2.41	0.50
2:B:392:GLN:O	2:B:395:ILE:HG22	2.11	0.50
2:B:396:PHE:CE2	2:B:405:ALA:HB2	2.46	0.50
1:C:397:TYR:CD1	1:C:420:LEU:HD11	2.46	0.50
2:D:236:LEU:C	2:D:268:LYS:HZ1	2.12	0.50
2:D:264:ASP:C	2:D:266:GLN:H	2.19	0.50
2:B:346:GLN:O	2:B:350:GLU:HG3	2.11	0.50
2:B:304:VAL:HG13	2:B:330:TYR:HE2	1.77	0.50
1:C:24:ARG:HD2	1:C:493:TRP:CZ2	2.46	0.50
1:C:329:LEU:HB3	1:C:333:LYS:NZ	2.27	0.50
1:A:244:GLU:OE1	1:A:426:ARG:NE	2.42	0.50
1:A:377:ASP:O	1:A:380:ARG:NE	2.44	0.50
2:B:78:VAL:HG22	2:B:79:ALA:H	1.76	0.50
2:B:254:TYR:CD2	2:B:271:HIS:HB2	2.46	0.50
1:C:241:VAL:HA	1:C:262:TYR:CE2	2.47	0.50
2:D:162:ILE:O	2:D:162:ILE:HG13	2.11	0.50
1:A:202:ARG:NH1	2:D:84:MSE:HE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:GLU:HB3	2:D:171:ARG:NH1	2.26	0.50
2:D:406:SER:HA	2:D:409:GLU:OE1	2.11	0.50
2:D:419:ARG:CG	2:D:423:GLN:NE2	2.75	0.50
2:B:84:MSE:HE1	1:C:227:VAL:HB	1.94	0.50
2:B:300:LEU:O	2:B:304:VAL:HG12	2.12	0.50
1:C:323:MSE:HB3	1:C:354:LEU:CB	2.42	0.50
1:C:435:ASP:HA	1:C:439:GLY:O	2.11	0.50
2:B:203:PHE:CE2	2:B:231:ASN:OD1	2.65	0.50
2:D:321:SER:O	2:D:325:LEU:HD12	2.12	0.50
1:A:390:ILE:N	1:A:390:ILE:HD12	2.27	0.49
1:C:138:ARG:NH2	1:C:146:ARG:NH1	2.59	0.49
1:C:494:THR:O	1:C:495:GLN:C	2.54	0.49
2:D:194:ILE:H	2:D:216:ASP:HB3	1.77	0.49
1:A:472:GLU:HA	1:A:475:GLN:CD	2.37	0.49
1:A:473:MSE:C	1:A:475:GLN:N	2.69	0.49
2:D:290:ILE:HB	2:D:314:ILE:HD13	1.93	0.49
2:D:407:ILE:HA	2:D:410:GLU:HB3	1.93	0.49
1:C:75:ALA:HB3	1:C:143:SER:OG	2.12	0.49
1:C:318:ARG:O	1:C:320:PRO:HD3	2.12	0.49
2:D:286:LYS:HZ1	2:D:310:LEU:HD11	1.76	0.49
1:C:270:ASP:OD2	1:C:271:LYS:HE3	2.12	0.49
1:A:449:VAL:CG1	1:A:452:GLN:NE2	2.66	0.49
2:B:348:TYR:CZ	2:B:369:LYS:HG2	2.47	0.49
1:C:339:VAL:O	1:C:342:THR:OG1	2.27	0.49
2:D:199:LEU:HD22	2:D:199:LEU:N	2.28	0.49
2:B:195:LEU:HB3	2:B:219:PHE:HE1	1.77	0.49
1:C:391:TYR:HB2	1:C:416:SER:OG	2.13	0.49
1:C:453:ILE:HD12	1:C:454:ILE:HG13	1.95	0.49
2:D:203:PHE:CZ	2:D:234:LEU:HD11	2.47	0.49
2:D:217:ILE:HD12	2:D:217:ILE:O	2.13	0.49
1:A:366:LEU:HD13	1:A:370:ILE:HD11	1.95	0.49
1:A:400:ALA:O	1:A:423:PHE:HE2	1.96	0.49
2:B:38:PRO:HG2	2:B:41:MSE:HE3	1.94	0.49
1:C:87:GLN:O	2:D:170:LEU:N	2.31	0.49
1:A:322:SER:HA	1:A:353:THR:O	2.12	0.49
2:B:363:VAL:HG12	2:B:364:LEU:HD12	1.94	0.49
2:D:15:LEU:HD11	2:D:219:PHE:CB	2.43	0.49
1:A:42:MSE:HE1	1:A:166:PHE:CZ	2.48	0.48
1:A:369:ARG:O	1:A:370:ILE:C	2.55	0.48
1:A:466:SER:CA	1:A:467:GLN:HE21	2.23	0.48
1:C:90:GLY:O	1:C:91:GLN:NE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:SER:C	1:C:333:LYS:NZ	2.70	0.48
1:C:420:LEU:O	1:C:421:ILE:HD13	2.12	0.48
2:D:46:THR:O	2:D:49:LEU:HD12	2.13	0.48
2:D:219:PHE:HD1	2:D:247:VAL:CG1	2.24	0.48
2:D:291:LEU:O	2:D:358:ASN:ND2	2.46	0.48
2:D:391:ALA:HB2	2:D:424:ALA:O	2.13	0.48
1:A:145:VAL:HG12	1:A:146:ARG:N	2.28	0.48
1:A:111:GLN:HB3	2:B:174:LYS:NZ	2.28	0.48
2:B:291:LEU:CD1	2:B:344:ILE:HD11	2.43	0.48
1:C:283:LYS:O	1:C:287:GLU:HB2	2.13	0.48
2:D:286:LYS:HZ1	2:D:310:LEU:CD1	2.25	0.48
2:D:338:ASN:N	2:D:338:ASN:HD22	2.12	0.48
2:D:390:ILE:O	2:D:428:HIS:ND1	2.47	0.48
1:A:349:LEU:HD13	1:A:350:PRO:N	2.29	0.48
1:A:371:GLU:HB3	1:A:375:ALA:O	2.13	0.48
2:B:203:PHE:HE2	2:B:231:ASN:ND2	2.11	0.48
2:B:363:VAL:HG12	2:B:364:LEU:CD1	2.43	0.48
2:D:210:THR:CG2	2:D:241:LEU:HG	2.43	0.48
2:D:291:LEU:CD1	2:D:344:ILE:HD11	2.43	0.48
1:C:44:LEU:HB3	1:C:141:TYR:CE1	2.49	0.48
1:C:322:SER:N	1:C:395:GLU:OE1	2.47	0.48
1:C:349:LEU:HB3	1:C:352:LEU:CD1	2.38	0.48
1:C:461:ILE:O	1:C:464:LEU:HG	2.13	0.48
2:D:309:GLN:NE2	2:D:309:GLN:H	2.11	0.48
1:A:481:ALA:O	1:A:484:TYR:N	2.38	0.48
1:C:111:GLN:CD	2:D:174:LYS:HZ1	2.20	0.48
1:C:161:LEU:HD21	1:C:164:ARG:NH1	2.27	0.48
1:C:423:PHE:HD2	1:C:442:LEU:HB2	1.79	0.48
1:A:245:HIS:CD2	1:A:286:LEU:HD13	2.48	0.48
2:B:280:ARG:NH2	2:B:348:TYR:O	2.47	0.48
2:B:353:ILE:HD13	2:B:355:LEU:HG	1.95	0.48
2:B:403:GLN:NE2	2:B:404:LEU:HA	2.29	0.48
1:C:323:MSE:HG2	1:C:354:LEU:HB3	1.94	0.48
1:C:350:PRO:O	1:C:352:LEU:HD12	2.13	0.48
1:A:285:ILE:O	1:A:289:GLN:HG3	2.14	0.48
1:A:414:VAL:HA	1:A:477:SER:HB3	1.95	0.48
2:B:220:TRP:CZ2	2:B:222:GLU:HB2	2.48	0.48
2:B:262:ALA:O	2:B:266:GLN:HG3	2.14	0.48
2:B:427:ARG:HH11	2:B:427:ARG:CG	2.26	0.48
1:A:27:ILE:HG21	1:A:493:TRP:CD1	2.49	0.48
2:B:220:TRP:HE1	2:B:224:LEU:CD1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:LEU:HD12	2:B:384:LEU:N	2.29	0.48
2:B:432:VAL:HB	2:B:436:LEU:HD23	1.96	0.48
2:D:164:THR:HG22	2:D:170:LEU:HB2	1.96	0.48
1:A:25:ALA:O	1:A:29:ARG:HG3	2.13	0.47
2:B:386:ASP:N	2:B:386:ASP:OD1	2.47	0.47
1:C:79:VAL:O	1:C:125:VAL:N	2.43	0.47
1:C:327:SER:C	1:C:333:LYS:HZ1	2.22	0.47
1:C:346:HIS:HD2	1:C:375:ALA:HB2	1.79	0.47
2:D:196:PHE:HZ	2:D:243:THR:HG21	1.79	0.47
2:D:224:LEU:HB2	2:D:256:LYS:NZ	2.29	0.47
1:A:338:LEU:CD1	1:A:400:ALA:HB2	2.39	0.47
1:A:359:LYS:HZ2	1:A:383:GLY:CA	2.26	0.47
1:C:81:LEU:HD12	1:C:123:ASP:O	2.15	0.47
2:D:224:LEU:CB	2:D:256:LYS:CE	2.93	0.47
2:D:5:PHE:HB2	2:D:30:VAL:HG12	1.96	0.47
1:C:23:TYR:CZ	1:C:27:ILE:HD11	2.50	0.47
1:C:239:VAL:HG11	1:C:265:GLN:HG2	1.97	0.47
2:D:336:TYR:CE1	2:D:347:LEU:HD21	2.49	0.47
1:A:367:ARG:HA	1:A:370:ILE:HG12	1.96	0.47
1:A:440:TYR:CE2	1:A:473:MSE:HE1	2.48	0.47
2:B:2:ILE:HG22	2:B:27:PRO:HG2	1.96	0.47
1:C:426:ARG:HB3	1:C:427:TYR:CG	2.49	0.47
2:D:244:GLN:CD	2:D:244:GLN:N	2.72	0.47
1:A:359:LYS:NZ	1:A:383:GLY:CA	2.77	0.47
2:D:419:ARG:HG3	2:D:423:GLN:NE2	2.29	0.47
1:A:145:VAL:HG12	1:A:146:ARG:H	1.78	0.47
1:A:470:GLN:HG3	1:A:471:GLN:H	1.80	0.47
2:B:118:GLU:HG2	2:B:129:LYS:HG2	1.96	0.47
2:B:203:PHE:O	2:B:206:SER:N	2.46	0.47
1:C:23:TYR:O	1:C:27:ILE:HD12	2.14	0.47
1:C:80:THR:HA	1:C:123:ASP:O	2.15	0.47
1:C:346:HIS:CD2	1:C:375:ALA:HB2	2.49	0.47
1:C:420:LEU:C	1:C:421:ILE:HD13	2.40	0.47
1:C:468:GLY:O	1:C:472:GLU:HG3	2.14	0.47
1:C:492:ALA:O	1:C:496:LEU:N	2.46	0.47
2:D:165:LEU:N	2:D:165:LEU:CD2	2.78	0.47
2:D:212:ARG:HG2	2:D:242:ARG:HH22	1.80	0.47
2:D:217:ILE:HG22	2:D:245:THR:HB	1.97	0.47
2:D:246:ILE:O	2:D:269:PHE:HA	2.14	0.47
2:D:324:LEU:HD23	2:D:324:LEU:C	2.40	0.47
1:C:117:LEU:HD11	1:C:124:PHE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:ASP:OD1	2:D:243:THR:HG22	2.15	0.47
1:A:256:ILE:HD11	1:A:289:GLN:NE2	2.30	0.47
1:A:354:LEU:C	1:A:354:LEU:HD12	2.40	0.47
1:A:367:ARG:CZ	1:A:368:ARG:HH12	2.27	0.47
1:A:454:ILE:HD12	1:A:454:ILE:H	1.80	0.47
2:B:271:HIS:ND1	2:B:272:LEU:N	2.63	0.47
2:D:154:GLU:OE2	2:D:176:ARG:NH1	2.48	0.47
1:A:359:LYS:HB2	1:A:384:HIS:CE1	2.50	0.47
1:C:328:ARG:NH2	1:C:359:LYS:N	2.60	0.47
1:C:117:LEU:HD12	1:C:125:VAL:HA	1.96	0.46
1:C:129:GLU:HB3	1:C:136:LEU:CD1	2.45	0.46
2:D:286:LYS:HD2	2:D:310:LEU:HD12	1.97	0.46
2:B:84:MSE:HE3	1:C:198:ALA:HB1	1.97	0.46
2:B:254:TYR:OH	2:B:258:MSE:HE2	2.15	0.46
2:B:288:ALA:N	2:B:311:VAL:O	2.47	0.46
2:B:403:GLN:O	2:B:405:ALA:N	2.49	0.46
1:A:363:GLU:C	1:A:366:LEU:H	2.23	0.46
1:A:464:LEU:HG	1:A:464:LEU:O	2.16	0.46
1:C:81:LEU:HD21	1:C:102:VAL:HG11	1.98	0.46
1:C:321:TYR:HB3	1:C:352:LEU:CD1	2.44	0.46
2:B:70:TRP:CZ3	2:B:88:ARG:HG3	2.50	0.46
2:B:317:LEU:HA	2:B:338:ASN:HA	1.97	0.46
2:D:302:THR:O	2:D:306:SER:OG	2.29	0.46
2:D:368:ARG:NH1	2:D:389:TYR:OH	2.49	0.46
1:A:295:ASP:C	1:A:296:LYS:HG2	2.41	0.46
1:A:337:TRP:CZ3	1:A:453:ILE:HD13	2.51	0.46
1:A:370:ILE:HG22	1:A:371:GLU:OE1	2.16	0.46
1:A:397:TYR:HD2	1:A:420:LEU:HD12	1.80	0.46
2:B:295:ASP:HB2	2:B:296:GLN:CA	2.45	0.46
1:C:26:GLN:HA	1:C:29:ARG:HH11	1.78	0.46
1:C:111:GLN:CD	2:D:174:LYS:NZ	2.73	0.46
2:D:315:ALA:HA	2:D:336:TYR:O	2.16	0.46
2:D:385:HIS:HA	2:D:386:ASP:C	2.40	0.46
1:A:361:SER:O	1:A:362:GLU:HB2	2.14	0.46
1:A:414:VAL:HG11	1:A:480:VAL:HG23	1.98	0.46
2:B:231:ASN:HA	2:B:234:LEU:HD13	1.97	0.46
1:C:12:TRP:CE2	1:C:46:ASP:OD1	2.66	0.46
1:C:311:LEU:H	1:C:311:LEU:HD12	1.79	0.46
2:D:254:TYR:HE2	2:D:269:PHE:HE1	1.63	0.46
1:A:283:LYS:O	1:A:287:GLU:HB2	2.15	0.46
2:B:257:ALA:HB1	2:B:269:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:LEU:HD21	2:B:394:HIS:CD2	2.47	0.45
2:B:378:LEU:CD2	2:B:394:HIS:HB3	2.46	0.45
1:C:352:LEU:HD21	1:C:465:PHE:CE2	2.51	0.45
2:D:28:THR:HG23	2:D:41:MSE:HA	1.98	0.45
1:A:334:HIS:CE1	1:A:337:TRP:CE2	3.04	0.45
1:A:376:GLN:O	1:A:379:ILE:HG22	2.16	0.45
1:C:407:GLY:HA3	1:C:410:LEU:HD22	1.98	0.45
2:D:35:GLY:HA3	2:D:121:ASN:HA	1.98	0.45
2:D:235:ILE:CD1	2:D:243:THR:O	2.65	0.45
2:D:412:LEU:HD12	2:D:417:GLN:CG	2.46	0.45
1:A:146:ARG:HD2	1:A:149:SER:OG	2.15	0.45
1:A:359:LYS:HZ2	1:A:383:GLY:C	2.24	0.45
1:A:382:LYS:NZ	1:A:385:ALA:HB2	2.32	0.45
2:B:289:LEU:O	2:B:290:ILE:HD13	2.16	0.45
1:C:323:MSE:O	1:C:324:ILE:HB	2.16	0.45
1:C:130:TYR:CE1	1:C:140:ASP:OD1	2.70	0.45
1:C:303:ILE:HG21	1:C:493:TRP:NE1	2.31	0.45
2:D:163:LEU:HD21	2:D:165:LEU:CD2	2.46	0.45
1:A:366:LEU:HD13	1:A:370:ILE:HD13	1.98	0.45
1:A:463:ALA:O	1:A:469:ARG:NH2	2.48	0.45
2:B:244:GLN:CD	2:B:268:LYS:HZ3	2.22	0.45
1:C:437:LYS:HA	1:C:437:LYS:HD2	1.71	0.45
1:C:494:THR:C	1:C:498:LYS:NZ	2.56	0.45
1:C:495:GLN:N	1:C:498:LYS:HZ1	2.12	0.45
2:B:292:THR:HA	2:B:358:ASN:HD22	1.81	0.45
1:C:499:GLU:OE2	1:C:499:GLU:N	2.44	0.45
2:D:286:LYS:HB2	2:D:286:LYS:HE2	1.83	0.45
2:B:251:LEU:H	2:B:430:ASN:ND2	2.10	0.45
2:B:336:TYR:CZ	2:B:347:LEU:HD21	2.51	0.45
1:A:417:GLY:HA3	1:A:478:TYR:CZ	2.52	0.45
2:B:64:VAL:HG21	2:B:91:ILE:HG12	1.98	0.45
1:C:408:LEU:O	1:C:411:MSE:HB3	2.17	0.45
2:D:194:ILE:H	2:D:216:ASP:CB	2.29	0.45
1:A:1:SER:HB3	1:A:213:ASP:OD2	2.17	0.45
1:A:359:LYS:HG3	1:A:384:HIS:CD2	2.51	0.45
1:A:128:VAL:HG23	1:A:142:PHE:HE2	1.82	0.44
1:A:464:LEU:HA	1:A:469:ARG:CZ	2.46	0.44
2:D:217:ILE:HD13	2:D:219:PHE:CE2	2.52	0.44
2:D:254:TYR:OH	2:D:258:MSE:SE	2.85	0.44
2:D:336:TYR:CD2	2:D:343:GLN:NE2	2.85	0.44
1:A:484:TYR:HA	1:A:488:ARG:CZ	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:HIS:CE1	1:C:289:GLN:HE22	2.30	0.44
2:D:196:PHE:CZ	2:D:243:THR:HG21	2.51	0.44
2:D:209:LEU:O	2:D:212:ARG:N	2.49	0.44
2:D:209:LEU:O	2:D:210:THR:C	2.61	0.44
1:A:344:GLN:N	1:A:344:GLN:OE1	2.50	0.44
1:A:367:ARG:HB3	1:A:368:ARG:HH11	1.81	0.44
2:B:344:ILE:HA	2:B:347:LEU:HD12	1.99	0.44
1:A:386:ASP:OD1	1:A:386:ASP:C	2.60	0.44
1:C:263:ASP:O	1:C:267:THR:OG1	2.27	0.44
1:C:323:MSE:CG	1:C:354:LEU:HB3	2.47	0.44
2:B:441:LEU:HD23	2:B:441:LEU:HA	1.73	0.44
1:C:306:GLY:C	1:C:411:MSE:HE3	2.42	0.44
2:D:224:LEU:CB	2:D:256:LYS:NZ	2.81	0.44
2:D:290:ILE:HD11	2:D:355:LEU:CB	2.39	0.44
1:A:463:ALA:C	1:A:469:ARG:NH2	2.69	0.44
2:B:427:ARG:CG	2:B:427:ARG:NH1	2.81	0.44
1:C:117:LEU:HD23	1:C:119:GLN:O	2.18	0.44
1:C:432:PHE:CE1	1:C:484:TYR:CE2	3.06	0.44
2:D:219:PHE:CD1	2:D:247:VAL:HG12	2.51	0.44
2:B:3:GLN:OE1	2:B:28:THR:OG1	2.30	0.44
2:B:7:TYR:O	2:B:12:THR:HG21	2.18	0.44
2:B:304:VAL:CG1	2:B:330:TYR:HE2	2.30	0.44
2:D:122:LYS:HG2	2:D:123:GLN:OE1	2.18	0.44
2:D:217:ILE:CD1	2:D:219:PHE:CE2	3.01	0.44
2:D:307:LEU:HD22	2:D:410:GLU:OE2	2.17	0.44
2:D:310:LEU:HB3	2:D:312:PHE:CE1	2.53	0.44
1:C:141:TYR:CB	1:C:147:TYR:HE1	2.31	0.44
1:C:324:ILE:HD11	1:C:357:TYR:CE2	2.53	0.44
1:C:329:LEU:HG	1:C:359:LYS:HA	1.99	0.44
2:D:108:LEU:HD23	2:D:114:LEU:HA	1.99	0.44
2:B:217:ILE:HG23	2:B:245:THR:HB	2.00	0.44
1:C:308:LEU:O	1:C:485:LEU:HB2	2.18	0.44
1:C:467:GLN:HB3	1:C:468:GLY:HA2	2.00	0.44
2:D:174:LYS:N	2:D:174:LYS:HD3	2.31	0.44
2:D:192:ASP:HB3	2:D:193:HIS:ND1	2.33	0.44
2:D:236:LEU:HA	2:D:268:LYS:NZ	2.33	0.44
1:A:256:ILE:HB	1:A:293:TYR:CD2	2.53	0.43
1:C:80:THR:OG1	1:C:82:ASP:HB2	2.18	0.43
2:D:151:ARG:NH1	4:D:501:HOH:O	2.49	0.43
2:D:301:ASP:O	2:D:305:GLN:OE1	2.36	0.43
1:A:462:ILE:CA	1:A:465:PHE:H	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:HIS:CD2	2:B:382:GLN:HE21	2.28	0.43
2:B:380:PHE:HB3	2:B:397:ASP:O	2.17	0.43
1:C:167:TYR:CE2	2:D:150:GLU:OE2	2.71	0.43
1:A:202:ARG:NH2	1:A:230:GLU:OE1	2.52	0.43
1:A:382:LYS:NZ	1:A:383:GLY:C	2.76	0.43
2:B:378:LEU:CD2	2:B:394:HIS:HD2	2.31	0.43
1:C:130:TYR:HE1	1:C:140:ASP:OD1	2.01	0.43
2:D:225:TYR:O	2:D:226:ASP:C	2.62	0.43
2:D:251:LEU:N	2:D:430:ASN:HD21	2.05	0.43
2:D:297:ILE:HD12	2:D:358:ASN:HB3	2.00	0.43
1:A:338:LEU:H	1:A:338:LEU:CD1	2.23	0.43
2:B:235:ILE:HD12	2:B:243:THR:OG1	2.19	0.43
1:A:335:ILE:HD13	1:A:366:LEU:HD21	2.00	0.43
2:B:191:LEU:HD22	2:B:194:ILE:HD11	1.99	0.43
1:C:141:TYR:HB2	1:C:147:TYR:HE1	1.84	0.43
1:C:387:LEU:HB2	1:C:390:ILE:HG12	2.00	0.43
1:C:406:PHE:HZ	1:C:411:MSE:HE2	1.83	0.43
1:C:436:GLY:O	1:C:437:LYS:C	2.61	0.43
1:C:469:ARG:HA	1:C:472:GLU:CD	2.44	0.43
2:D:217:ILE:C	2:D:217:ILE:CD1	2.91	0.43
2:D:362:GLN:CB	2:D:384:LEU:HD21	2.40	0.43
2:D:377:ILE:O	2:D:378:LEU:HD23	2.18	0.43
2:B:295:ASP:OD1	2:B:321:SER:OG	2.33	0.43
1:C:408:LEU:HD23	1:C:408:LEU:HA	1.65	0.43
1:C:426:ARG:HA	1:C:427:TYR:HA	1.61	0.43
1:A:282:GLN:HG3	1:A:427:TYR:CZ	2.54	0.43
1:C:324:ILE:HG13	1:C:355:ASP:O	2.19	0.43
2:D:250:ASP:HA	2:D:430:ASN:ND2	2.33	0.43
1:A:151:TYR:CE1	2:B:153:VAL:HG11	2.53	0.43
1:A:370:ILE:HD12	1:A:370:ILE:HG23	1.70	0.43
1:A:404:GLU:OE2	1:A:406:PHE:O	2.37	0.43
1:A:414:VAL:CG2	1:A:420:LEU:HD21	2.47	0.43
1:A:440:TYR:CD1	1:A:460:LYS:HB3	2.52	0.43
2:B:196:PHE:CZ	2:B:243:THR:HG21	2.54	0.43
2:B:378:LEU:CD2	2:B:394:HIS:CD2	3.02	0.43
2:D:227:GLU:CD	2:D:228:LEU:HB2	2.43	0.43
2:D:272:LEU:HD21	2:D:436:LEU:HD22	1.97	0.43
2:B:94:ALA:HB2	2:B:103:LYS:HB2	2.01	0.43
2:B:212:ARG:HD3	2:B:242:ARG:NH1	2.34	0.43
1:A:357:TYR:HD1	1:A:387:LEU:HD11	1.82	0.43
1:A:366:LEU:HD12	1:A:381:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:LEU:CA	2:D:189:LEU:HD21	2.41	0.43
2:D:298:GLU:N	2:D:357:ILE:HG22	2.33	0.43
1:A:188:ARG:NH1	1:A:189:PHE:O	2.52	0.42
1:A:192:ARG:NH1	1:A:203:TYR:CE1	2.87	0.42
1:A:250:ALA:HB3	1:A:257:LEU:HD23	2.01	0.42
1:A:465:PHE:O	1:A:467:GLN:NE2	2.52	0.42
1:A:469:ARG:O	1:A:473:MSE:N	2.52	0.42
2:B:5:PHE:HA	2:B:197:ASN:OD1	2.18	0.42
1:C:17:VAL:HG11	1:C:220:ARG:HE	1.83	0.42
1:C:181:ASP:CB	1:C:183:GLN:HE21	2.28	0.42
1:C:365:LYS:O	1:C:368:ARG:HB2	2.19	0.42
2:D:305:GLN:O	2:D:308:PRO:HD3	2.19	0.42
2:B:150:GLU:O	2:B:164:THR:HG23	2.18	0.42
2:D:224:LEU:C	2:D:256:LYS:NZ	2.74	0.42
2:D:355:LEU:HB3	2:D:357:ILE:HG12	2.02	0.42
1:A:259:ASN:HD22	1:A:259:ASN:C	2.27	0.42
2:B:403:GLN:O	2:B:406:SER:N	2.42	0.42
1:C:478:TYR:N	1:C:478:TYR:CD1	2.86	0.42
2:D:220:TRP:O	2:D:249:PRO:HD2	2.19	0.42
2:D:246:ILE:O	2:D:269:PHE:HB2	2.20	0.42
1:A:23:TYR:HD1	1:A:305:VAL:O	2.02	0.42
2:B:134:SER:C	2:B:136:GLN:H	2.27	0.42
2:B:261:ALA:HB3	2:B:266:GLN:HG2	2.01	0.42
2:B:288:ALA:HA	2:B:353:ILE:HD11	2.01	0.42
1:C:81:LEU:HG	1:C:125:VAL:CG2	2.49	0.42
1:C:167:TYR:CZ	2:D:150:GLU:OE2	2.73	0.42
2:D:8:TYR:CD1	2:D:8:TYR:C	2.97	0.42
2:D:44:PRO:HB3	2:D:183:PHE:CG	2.55	0.42
2:D:244:GLN:CD	2:D:244:GLN:H	2.28	0.42
2:D:314:ILE:HG21	2:D:324:LEU:HD11	2.01	0.42
2:B:89:ALA:HB2	2:B:107:TRP:CE3	2.55	0.42
2:B:195:LEU:HB3	2:B:219:PHE:CE1	2.55	0.42
2:B:314:ILE:HB	2:B:335:LEU:CD2	2.48	0.42
1:C:391:TYR:O	1:C:418:LEU:HD11	2.19	0.42
2:D:194:ILE:CD1	2:D:242:ARG:HH11	2.32	0.42
1:A:363:GLU:C	1:A:365:LYS:N	2.75	0.42
1:A:367:ARG:HA	1:A:370:ILE:CG1	2.50	0.42
1:A:464:LEU:HA	1:A:469:ARG:NE	2.35	0.42
2:B:44:PRO:HB3	2:B:183:PHE:CG	2.55	0.42
2:B:422:LEU:N	2:B:422:LEU:HD23	2.34	0.42
2:D:210:THR:HG22	2:D:241:LEU:HG	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:ARG:HE	2:D:285:ARG:HB2	1.21	0.42
1:A:464:LEU:HD12	1:A:469:ARG:NE	2.35	0.42
2:B:298:GLU:HB2	2:B:359:HIS:CE1	2.54	0.42
1:C:338:LEU:N	1:C:338:LEU:HD22	2.34	0.42
2:D:19:LEU:HD12	2:D:20:LEU:N	2.35	0.42
2:D:51:ASP:OD2	2:D:125:ARG:NH1	2.53	0.42
2:D:180:ILE:O	2:D:184:LEU:HG	2.19	0.42
2:D:236:LEU:HA	2:D:268:LYS:CE	2.50	0.42
2:D:377:ILE:HG13	2:D:425:GLN:HE22	1.84	0.42
1:A:334:HIS:CD2	1:A:336:ASP:OD2	2.73	0.42
1:A:359:LYS:NZ	1:A:384:HIS:N	2.44	0.42
1:A:366:LEU:CD1	1:A:370:ILE:CD1	2.97	0.42
1:C:66:TYR:CD2	1:C:177:MSE:HE1	2.54	0.42
1:C:329:LEU:HD21	1:C:363:GLU:OE1	2.19	0.42
1:C:362:GLU:HG3	1:C:365:LYS:CD	2.49	0.42
1:C:437:LYS:CD	1:C:476:HIS:CD2	3.02	0.42
2:D:47:TYR:CD1	2:D:47:TYR:C	2.97	0.42
2:D:263:ALA:HA	2:D:266:GLN:HG3	2.02	0.42
2:D:270:LEU:C	2:D:271:HIS:ND1	2.78	0.42
2:D:400:GLN:HB2	2:D:401:PRO:CD	2.50	0.42
2:D:419:ARG:CG	2:D:423:GLN:HE22	2.33	0.42
2:B:107:TRP:NE1	2:B:118:GLU:OE2	2.50	0.42
2:B:215:GLN:HA	2:B:242:ARG:O	2.20	0.42
1:C:8:LEU:HD11	1:C:222:THR:HB	2.02	0.42
2:D:9:ASN:OD1	2:D:11:GLU:HG2	2.20	0.42
1:C:24:ARG:CD	1:C:493:TRP:CZ2	3.03	0.42
1:C:453:ILE:CD1	1:C:454:ILE:HG13	2.50	0.42
2:D:307:LEU:HD13	2:D:310:LEU:CD2	2.46	0.42
1:A:397:TYR:HB3	1:A:420:LEU:HD13	2.00	0.41
1:A:426:ARG:HA	1:A:427:TYR:HA	1.74	0.41
1:C:391:TYR:O	1:C:394:TYR:HB2	2.20	0.41
1:C:490:GLU:O	1:C:494:THR:HB	2.19	0.41
2:D:297:ILE:CG1	2:D:300:LEU:HD23	2.50	0.41
1:A:311:LEU:HD23	1:A:415:GLY:O	2.20	0.41
1:C:483:ASN:HA	1:C:488:ARG:HD3	2.02	0.41
2:D:419:ARG:HG2	2:D:423:GLN:NE2	2.35	0.41
1:A:33:GLN:OE1	1:A:501:ARG:NH1	2.40	0.41
2:B:1:MSE:HE2	2:B:195:LEU:CD1	2.44	0.41
1:C:6:ILE:HB	1:C:218:LEU:HD12	2.02	0.41
1:C:29:ARG:HH21	1:C:58:LEU:HG	1.84	0.41
2:D:223:PRO:HG2	2:D:225:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:TYR:C	2:D:256:LYS:N	2.76	0.41
1:A:157:ASP:O	1:A:157:ASP:OD1	2.38	0.41
1:A:202:ARG:O	1:A:206:GLN:HG3	2.21	0.41
2:B:59:LEU:HD23	2:B:59:LEU:HA	1.87	0.41
2:B:299:GLY:O	2:B:302:THR:OG1	2.33	0.41
1:C:22:ALA:O	1:C:26:GLN:HG3	2.20	0.41
1:C:282:GLN:HG3	1:C:427:TYR:CZ	2.55	0.41
1:C:285:ILE:HA	1:C:288:GLN:OE1	2.21	0.41
2:D:64:VAL:HG11	2:D:105:VAL:HG21	2.01	0.41
2:D:272:LEU:HD23	2:D:272:LEU:HA	1.94	0.41
2:D:295:ASP:CB	2:D:296:GLN:HA	2.45	0.41
1:A:357:TYR:OH	1:A:394:TYR:OH	2.37	0.41
2:B:238:ASN:OD1	2:B:240:GLN:N	2.44	0.41
2:B:397:ASP:HB2	2:B:400:GLN:HB2	2.03	0.41
1:C:31:ILE:O	1:C:32:GLN:HB2	2.21	0.41
1:C:497:LEU:HB3	1:C:501:ARG:NH1	2.36	0.41
1:A:21:GLN:NE2	1:A:219:ASP:OD2	2.54	0.41
1:C:335:ILE:HB	1:C:338:LEU:HB2	2.02	0.41
2:D:272:LEU:HD23	2:D:436:LEU:CD2	2.37	0.41
2:D:378:LEU:HD11	2:D:409:GLU:HB3	2.03	0.41
1:A:281:ALA:O	1:A:285:ILE:HG12	2.21	0.41
2:B:228:LEU:HD13	2:B:232:MSE:HG2	2.03	0.41
2:B:272:LEU:CD1	2:B:273:GLY:N	2.57	0.41
1:C:21:GLN:HG2	1:C:24:ARG:NH1	2.36	0.41
1:A:335:ILE:HD13	1:A:366:LEU:CD2	2.50	0.41
1:A:357:TYR:CE2	1:A:382:LYS:HB3	2.56	0.41
2:B:413:CYS:N	2:B:417:GLN:OE1	2.54	0.41
2:D:227:GLU:OE1	2:D:228:LEU:HB2	2.21	0.41
2:D:297:ILE:HG22	2:D:357:ILE:CG2	2.50	0.41
1:A:173:VAL:HG21	2:B:144:TYR:CE2	2.54	0.41
1:A:338:LEU:HA	1:A:341:ALA:HB3	2.02	0.41
1:A:465:PHE:C	1:A:469:ARG:HH22	2.28	0.41
1:A:465:PHE:HA	1:A:467:GLN:HE22	1.85	0.41
1:A:488:ARG:NH2	1:A:489:VAL:HG22	2.35	0.41
2:B:125:ARG:NH1	2:B:145:SER:C	2.77	0.41
2:B:253:THR:O	2:B:257:ALA:N	2.48	0.41
2:B:348:TYR:CE1	2:B:369:LYS:HG2	2.56	0.41
1:C:321:TYR:HB3	1:C:352:LEU:HD12	2.03	0.41
1:C:324:ILE:HD11	1:C:357:TYR:CD2	2.56	0.41
1:C:365:LYS:HA	1:C:368:ARG:HG3	2.03	0.41
2:D:163:LEU:HD13	2:D:179:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:SER:HB2	2:D:216:ASP:OD2	2.20	0.41
2:D:235:ILE:HA	2:D:235:ILE:HD12	1.75	0.41
1:A:321:TYR:N	1:A:395:GLU:OE2	2.51	0.41
1:A:337:TRP:HZ3	1:A:423:PHE:CZ	2.39	0.41
1:A:397:TYR:CD2	1:A:420:LEU:HD12	2.56	0.41
2:B:123:GLN:OE1	2:B:123:GLN:N	2.51	0.41
2:B:354:TYR:O	2:B:377:ILE:HA	2.21	0.41
1:C:321:TYR:CD2	1:C:350:PRO:HG2	2.56	0.41
2:D:246:ILE:O	2:D:269:PHE:CB	2.69	0.41
2:D:291:LEU:CD2	2:D:315:ALA:HB3	2.51	0.41
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.77	0.40
1:A:364:ASP:HB3	1:A:368:ARG:NH2	2.36	0.40
1:A:460:LYS:HD3	1:A:463:ALA:HB3	2.03	0.40
1:A:469:ARG:O	1:A:473:MSE:HG3	2.21	0.40
2:B:163:LEU:HD11	2:B:165:LEU:HD21	2.03	0.40
2:D:264:ASP:O	2:D:267:GLN:NE2	2.51	0.40
1:A:11:GLY:N	1:A:14:SER:HB2	2.34	0.40
1:A:470:GLN:CG	1:A:471:GLN:N	2.83	0.40
1:C:136:LEU:O	1:C:152:PHE:HB2	2.21	0.40
1:C:318:ARG:HH22	1:C:471:GLN:NE2	2.19	0.40
2:D:209:LEU:O	2:D:211:GLY:N	2.53	0.40
2:D:220:TRP:HD1	2:D:248:ILE:HG23	1.86	0.40
1:A:84:VAL:O	1:A:88:VAL:HG23	2.21	0.40
1:C:187:TYR:CD2	1:C:200:LEU:HD12	2.56	0.40
1:C:498:LYS:HD2	1:C:498:LYS:N	2.29	0.40
2:D:1:MSE:HE2	2:D:195:LEU:HD11	2.04	0.40
2:D:246:ILE:O	2:D:269:PHE:CA	2.69	0.40
2:D:341:LEU:HD23	2:D:341:LEU:HA	1.86	0.40
1:A:421:ILE:HD12	1:A:440:TYR:HB2	2.03	0.40
1:A:466:SER:N	1:A:467:GLN:HE21	2.20	0.40
2:D:255:GLU:CD	2:D:256:LYS:H	2.29	0.40
2:D:373:ASN:HB2	2:D:375:LEU:HD23	2.03	0.40
1:A:108:GLN:H	1:A:108:GLN:CD	2.29	0.40
1:A:195:TYR:CE2	2:B:109:ASP:HA	2.56	0.40
1:A:449:VAL:CG1	1:A:452:GLN:HE22	2.32	0.40
2:B:359:HIS:CD2	2:B:382:GLN:NE2	2.83	0.40
1:C:28:LEU:HA	1:C:28:LEU:HD23	1.80	0.40
1:C:50:HIS:CE1	1:C:118:ARG:HD2	2.56	0.40
1:C:99:GLY:C	1:C:120:GLU:HG3	2.47	0.40
2:D:168:GLU:OE2	2:D:186:ARG:NH2	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	501/503 (100%)	482 (96%)	16 (3%)	3 (1%)	21	50
1	C	501/503 (100%)	480 (96%)	21 (4%)	0	100	100
2	B	445/447 (100%)	418 (94%)	26 (6%)	1 (0%)	43	71
2	D	443/447 (99%)	413 (93%)	30 (7%)	0	100	100
All	All	1890/1900 (100%)	1793 (95%)	93 (5%)	4 (0%)	43	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	GLU
1	A	474	SER
1	A	370	ILE
2	B	78	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	435/429 (101%)	427 (98%)	8 (2%)	51	79
1	C	435/429 (101%)	431 (99%)	4 (1%)	70	88
2	B	392/384 (102%)	390 (100%)	2 (0%)	81	93
2	D	392/384 (102%)	385 (98%)	7 (2%)	51	79
All	All	1654/1626 (102%)	1633 (99%)	21 (1%)	61	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	GLU
1	A	95	SER
1	A	184	GLU
1	A	222	THR
1	A	230	GLU
1	A	296	LYS
1	A	334	HIS
1	A	386	ASP
2	B	12	THR
2	B	363	VAL
1	C	95	SER
1	C	147	TYR
1	C	233	GLN
1	C	434	ASP
2	D	49	LEU
2	D	136	GLN
2	D	242	ARG
2	D	306	SER
2	D	311	VAL
2	D	349	LEU
2	D	376	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	83	GLN
1	A	127	HIS
1	A	206	GLN
1	A	249	ASN
1	A	259	ASN
1	A	288	GLN
1	A	291	GLN
1	A	334	HIS
1	A	376	GLN
1	A	467	GLN
1	A	470	GLN
1	A	476	HIS
2	B	231	ASN
2	B	359	HIS
2	B	362	GLN

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Mol	Chain	Res	Type
2	B	382	GLN
2	B	392	GLN
2	B	403	GLN
2	B	430	ASN
1	C	33	GLN
1	C	67	ASN
1	C	83	GLN
1	C	122	GLN
1	C	163	GLN
1	C	183	GLN
1	C	206	GLN
1	C	209	GLN
1	C	211	GLN
1	C	233	GLN
1	C	242	HIS
1	C	245	HIS
1	C	289	GLN
1	C	430	GLN
1	C	475	GLN
1	C	476	HIS
1	C	483	ASN
1	C	495	GLN
2	D	13	GLN
2	D	92	HIS
2	D	309	GLN
2	D	338	ASN
2	D	388	HIS
2	D	394	HIS
2	D	430	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	497/503 (98%)	0.53	74 (14%) 5 4	11, 51, 121, 141	0
1	C	497/503 (98%)	1.30	139 (27%) 1 1	22, 71, 119, 141	0
2	B	439/447 (98%)	0.76	58 (13%) 7 6	14, 62, 105, 131	0
2	D	437/447 (97%)	1.14	94 (21%) 2 2	15, 77, 118, 161	0
All	All	1870/1900 (98%)	0.93	365 (19%) 3 3	11, 67, 117, 161	0

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	381	LEU	8.0
2	D	407	ILE	5.8
1	C	352	LEU	5.5
1	C	311	LEU	5.5
1	C	322	SER	5.4
1	C	325	THR	5.3
1	C	375	ALA	5.3
2	D	251	LEU	5.2
2	D	402	ALA	5.1
1	C	484	TYR	5.0
1	C	474	SER	4.9
2	D	234	LEU	4.8
1	C	383	GLY	4.7
1	C	357	TYR	4.7
1	C	328	ARG	4.6
2	D	382	GLN	4.5
2	D	445	LEU	4.5
1	C	380	ARG	4.5
2	B	407	ILE	4.5
1	C	315	LYS	4.5
1	C	317	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
2	D	384	LEU	4.4
1	A	338	LEU	4.3
1	C	354	LEU	4.3
1	C	378	TYR	4.3
1	C	318	ARG	4.3
2	D	20	LEU	4.3
1	C	464	LEU	4.3
2	D	286	LYS	4.3
1	C	448	HIS	4.2
1	C	350	PRO	4.2
2	B	406	SER	4.2
1	C	314	PRO	4.2
1	C	397	TYR	4.2
2	B	401	PRO	4.2
1	C	363	GLU	4.2
1	A	317	PRO	4.1
1	A	448	HIS	4.1
1	C	320	PRO	4.1
1	C	374	GLY	4.1
1	C	384	HIS	4.0
2	B	385	HIS	3.9
2	B	398	SER	3.9
2	D	211	GLY	3.9
2	D	411	ALA	3.9
1	C	90	GLY	3.8
1	C	335	ILE	3.8
2	D	385	HIS	3.8
1	C	346	HIS	3.8
1	C	465	PHE	3.8
2	D	236	LEU	3.8
2	D	328	LEU	3.8
1	C	331	THR	3.7
1	C	326	ALA	3.7
2	D	404	LEU	3.7
1	A	329	LEU	3.7
1	C	324	ILE	3.7
1	C	438	ASN	3.6
1	C	379	ILE	3.6
2	B	208	SER	3.6
1	C	382	LYS	3.6
1	C	432	PHE	3.6
2	D	437	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	328	ARG	3.6
2	D	270	LEU	3.6
2	D	365	GLN	3.5
1	C	339	VAL	3.5
2	D	330	TYR	3.5
2	B	415	VAL	3.5
2	B	302	THR	3.5
1	A	380	ARG	3.5
1	C	476	HIS	3.5
1	C	477	SER	3.4
2	D	399	SER	3.4
1	A	465	PHE	3.4
1	C	396	LEU	3.4
1	A	369	ARG	3.4
1	C	355	ASP	3.4
2	B	225	TYR	3.4
2	B	97	ALA	3.4
2	D	362	GLN	3.4
2	D	383	THR	3.4
1	C	329	LEU	3.3
2	D	412	LEU	3.3
1	C	316	GLU	3.3
1	C	332	GLU	3.3
1	C	330	ALA	3.3
1	C	359	LYS	3.3
1	A	460	LYS	3.3
1	A	331	THR	3.3
1	C	343	VAL	3.3
1	C	449	VAL	3.3
2	D	403	GLN	3.3
1	C	440	TYR	3.2
1	C	123	ASP	3.2
1	C	348	GLN	3.2
1	A	184	GLU	3.2
1	C	351	GLU	3.2
1	C	446	SER	3.2
1	C	467	GLN	3.2
1	A	382	LYS	3.2
1	C	418	LEU	3.2
2	B	411	ALA	3.2
1	C	402	THR	3.2
1	C	395	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	347	ALA	3.2
2	D	262	ALA	3.2
2	B	331	LYS	3.2
1	A	370	ILE	3.2
1	C	419	PRO	3.2
2	D	395	ILE	3.2
1	C	420	LEU	3.1
2	D	254	TYR	3.1
1	A	360	GLY	3.1
1	A	453	ILE	3.1
1	C	462	ILE	3.1
1	A	365	LYS	3.1
1	C	403	SER	3.1
2	D	252	ALA	3.1
2	B	192	ASP	3.1
1	C	353	THR	3.1
1	C	369	ARG	3.1
1	C	345	ALA	3.1
1	A	503	ASP	3.1
1	C	503	ASP	3.1
1	C	337	TRP	3.1
2	D	264	ASP	3.1
1	C	481	ALA	3.0
2	B	288	ALA	3.0
1	A	449	VAL	3.0
2	B	396	PHE	3.0
1	A	445	SER	3.0
1	C	445	SER	3.0
1	A	367	ARG	3.0
1	C	370	ILE	3.0
2	D	267	GLN	3.0
1	A	349	LEU	3.0
1	C	362	GLU	3.0
1	C	310	GLN	3.0
1	C	349	LEU	3.0
1	C	393	GLY	3.0
2	D	409	GLU	3.0
2	D	235	ILE	2.9
1	C	391	TYR	2.9
2	D	410	GLU	2.9
1	C	312	THR	2.9
1	C	342	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	421	ILE	2.9
1	A	383	GLY	2.9
2	D	296	GLN	2.9
2	D	398	SER	2.9
2	D	19	LEU	2.9
1	A	334	HIS	2.9
2	D	245	THR	2.9
2	B	317	LEU	2.9
1	A	377	ASP	2.8
1	C	386	ASP	2.8
2	D	215	GLN	2.8
1	A	378	TYR	2.8
2	B	404	LEU	2.8
2	D	406	SER	2.8
1	C	321	TYR	2.8
2	D	405	ALA	2.8
1	C	85	LEU	2.8
2	D	265	GLN	2.8
2	D	47	TYR	2.8
2	D	218	LEU	2.8
1	C	333	LYS	2.8
1	C	87	GLN	2.7
1	A	393	GLY	2.7
2	B	309	GLN	2.7
1	A	347	ALA	2.7
1	C	113	ILE	2.7
1	C	389	GLN	2.7
1	A	339	VAL	2.7
2	B	234	LEU	2.7
2	B	297	ILE	2.7
1	C	367	ARG	2.7
1	C	401	SER	2.7
2	D	408	LEU	2.7
2	D	219	PHE	2.7
1	C	365	LYS	2.7
2	D	253	THR	2.7
1	A	310	GLN	2.7
1	C	361	SER	2.7
2	D	396	PHE	2.6
1	A	337	TRP	2.6
1	A	23	TYR	2.6
1	A	358	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	415	GLY	2.6
1	C	398	LEU	2.6
2	B	310	LEU	2.6
2	D	415	VAL	2.6
1	A	466	SER	2.6
2	D	329	SER	2.6
1	A	488	ARG	2.6
2	D	322	PRO	2.6
1	A	315	LYS	2.6
1	C	356	ILE	2.6
2	B	443	SER	2.6
2	B	271	HIS	2.6
1	A	320	PRO	2.6
1	C	414	VAL	2.6
2	D	310	LEU	2.6
1	C	482	GLU	2.6
2	D	246	ILE	2.6
2	B	231	ASN	2.6
1	A	384	HIS	2.6
1	A	468	GLY	2.6
2	B	270	LEU	2.6
2	B	413	CYS	2.6
1	C	447	ASN	2.6
2	D	391	ALA	2.6
1	A	355	ASP	2.6
2	D	271	HIS	2.5
1	C	388	SER	2.5
1	A	352	LEU	2.5
2	D	209	LEU	2.5
2	D	297	ILE	2.5
1	A	330	ALA	2.5
1	A	341	ALA	2.5
2	D	261	ALA	2.5
1	A	381	LEU	2.5
2	B	325	LEU	2.5
2	B	389	TYR	2.5
1	A	314	PRO	2.5
1	C	408	LEU	2.5
1	C	400	ALA	2.5
2	B	286	LYS	2.5
1	A	464	LEU	2.5
1	C	338	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	217	ILE	2.5
1	A	332	GLU	2.5
1	C	423	PHE	2.5
1	C	478	TYR	2.5
1	C	463	ALA	2.5
2	B	402	ALA	2.5
2	D	343	GLN	2.5
1	A	325	THR	2.5
2	D	243	THR	2.5
2	D	379	GLY	2.4
2	D	206	SER	2.4
1	A	457	PHE	2.4
2	D	227	GLU	2.4
1	C	32	GLN	2.4
2	D	225	TYR	2.4
2	D	260	LEU	2.4
2	D	324	LEU	2.4
2	B	395	ILE	2.4
1	C	468	GLY	2.4
1	A	373	ALA	2.4
1	A	376	GLN	2.4
1	C	471	GLN	2.4
1	C	479	GLN	2.4
2	B	24	TYR	2.4
2	B	393	GLN	2.4
2	D	244	GLN	2.4
1	A	350	PRO	2.4
2	B	353	ILE	2.4
1	C	319	LYS	2.4
2	D	269	PHE	2.4
2	B	296	GLN	2.4
1	C	313	TYR	2.4
2	D	275	HIS	2.4
2	D	401	PRO	2.4
2	D	414	GLY	2.4
2	D	413	CYS	2.4
1	A	351	GLU	2.4
1	A	392	ALA	2.4
1	C	340	ALA	2.4
2	D	357	ILE	2.4
1	C	410	LEU	2.3
1	A	359	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	444	VAL	2.3
1	C	457	PHE	2.3
1	C	82	ASP	2.3
2	B	263	ALA	2.3
1	C	334	HIS	2.3
2	B	256	LYS	2.3
2	D	433	PRO	2.3
2	D	334	VAL	2.3
2	D	358	ASN	2.3
2	B	405	ALA	2.3
1	C	475	GLN	2.3
2	B	240	GLN	2.3
1	C	416	SER	2.3
2	B	380	PHE	2.3
1	C	373	ALA	2.3
2	B	213	ALA	2.3
1	C	461	ILE	2.3
2	B	394	HIS	2.3
2	D	248	ILE	2.3
1	C	307	SER	2.3
2	D	201	TYR	2.3
1	C	480	VAL	2.3
1	C	306	GLY	2.3
1	C	499	GLU	2.2
2	B	287	ASP	2.2
2	D	419	ARG	2.2
2	B	253	THR	2.2
1	A	316	GLU	2.2
2	D	97	ALA	2.2
2	D	303	LEU	2.2
1	A	344	GLN	2.2
2	D	394	HIS	2.2
1	A	361	SER	2.2
1	C	104	TYR	2.2
1	C	327	SER	2.2
1	A	326	ALA	2.2
1	C	437	LYS	2.2
1	C	455	ALA	2.2
2	B	328	LEU	2.2
2	D	189	LEU	2.2
2	B	212	ARG	2.2
2	B	397	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	294	SER	2.2
1	C	392	ALA	2.2
2	B	52	GLU	2.2
2	D	213	ALA	2.2
2	D	257	ALA	2.2
2	D	416	GLU	2.2
1	C	13	ALA	2.2
1	C	341	ALA	2.2
1	C	368	ARG	2.1
2	D	194	ILE	2.1
2	B	382	GLN	2.1
2	D	268	LYS	2.1
1	C	407	GLY	2.1
1	A	366	LEU	2.1
2	D	259	SER	2.1
1	A	459	GLU	2.1
2	B	403	GLN	2.1
1	A	436	GLY	2.1
1	C	105	PHE	2.1
2	D	22	ALA	2.1
1	A	327	SER	2.1
1	A	421	ILE	2.1
1	C	452	GLN	2.1
2	B	305	GLN	2.1
2	B	442	GLN	2.1
2	D	423	GLN	2.1
1	A	444	VAL	2.1
1	A	451	ASP	2.1
1	C	485	LEU	2.1
2	D	378	LEU	2.1
1	A	375	ALA	2.1
1	A	456	ALA	2.1
1	A	313	TYR	2.1
2	D	134	SER	2.1
1	A	452	GLN	2.1
1	C	436	GLY	2.1
1	C	336	ASP	2.1
2	D	301	ASP	2.1
2	B	339	ALA	2.1
1	C	458	VAL	2.0
2	B	357	ILE	2.0
1	A	362	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	14	SER	2.0
1	A	354	LEU	2.0
2	B	307	LEU	2.0
2	B	422	LEU	2.0
1	C	358	GLY	2.0
2	B	264	ASP	2.0
1	A	319	LYS	2.0
1	A	391	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	601	1/1	0.98	0.19	14,14,14,14	0
3	MG	B	501	1/1	0.99	0.24	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.