



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:24 AM UTC

PDB ID : 4KSA / pdb_00004ksa
Title : Crystal Structure of Malonyl-CoA decarboxylase from Rhodopseudomonas palustris, Northeast Structural Genomics Consortium Target RpR127
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Deposited on : 2013-05-17
Resolution : 2.70 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

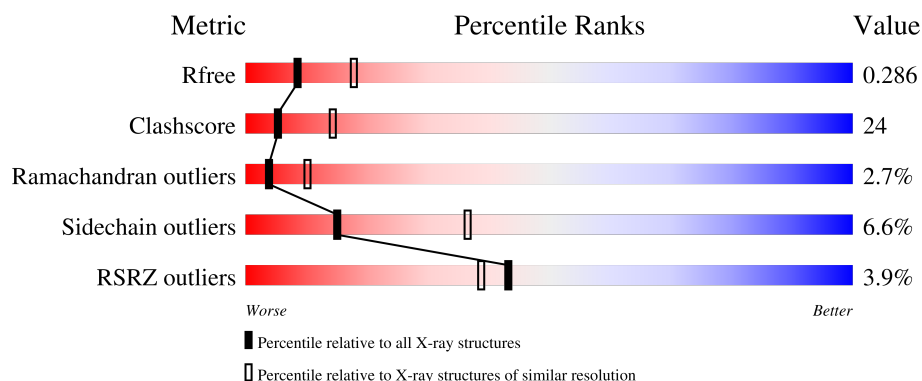
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	453	2% 56% 35% 5% .
1	B	453	6% 48% 37% 5% 9%
1	C	453	4% 53% 40% . .
1	D	453	3% 49% 36% 6% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13442 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 Malonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	Se	0	0	0
			3405	2151	611	638	1	4			
1	B	411	Total	C	N	O	S	Se	0	0	0
			3208	2031	574	598	1	4			
1	C	436	Total	C	N	O	S	Se	0	0	0
			3398	2147	610	636	1	4			
1	D	413	Total	C	N	O	S	Se	0	0	0
			3222	2041	576	600	1	4			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MSE	-	initiating methionine	UNP Q6NCB2
A	452	LEU	-	expression tag	UNP Q6NCB2
A	453	GLU	-	expression tag	UNP Q6NCB2
A	454	HIS	-	expression tag	UNP Q6NCB2
A	455	HIS	-	expression tag	UNP Q6NCB2
A	456	HIS	-	expression tag	UNP Q6NCB2
A	457	HIS	-	expression tag	UNP Q6NCB2
A	458	HIS	-	expression tag	UNP Q6NCB2
A	459	HIS	-	expression tag	UNP Q6NCB2
B	7	MSE	-	initiating methionine	UNP Q6NCB2
B	452	LEU	-	expression tag	UNP Q6NCB2
B	453	GLU	-	expression tag	UNP Q6NCB2
B	454	HIS	-	expression tag	UNP Q6NCB2
B	455	HIS	-	expression tag	UNP Q6NCB2
B	456	HIS	-	expression tag	UNP Q6NCB2
B	457	HIS	-	expression tag	UNP Q6NCB2
B	458	HIS	-	expression tag	UNP Q6NCB2
B	459	HIS	-	expression tag	UNP Q6NCB2
C	7	MSE	-	initiating methionine	UNP Q6NCB2
C	452	LEU	-	expression tag	UNP Q6NCB2
C	453	GLU	-	expression tag	UNP Q6NCB2

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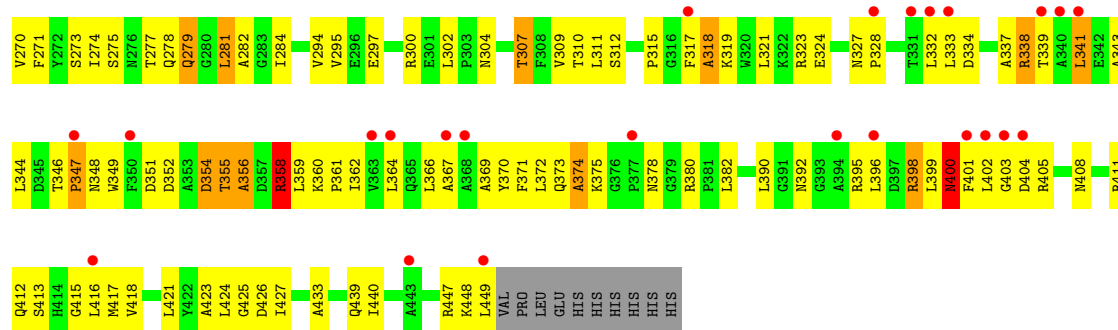
Chain	Residue	Modelled	Actual	Comment	Reference
C	454	HIS	-	expression tag	UNP Q6NCB2
C	455	HIS	-	expression tag	UNP Q6NCB2
C	456	HIS	-	expression tag	UNP Q6NCB2
C	457	HIS	-	expression tag	UNP Q6NCB2
C	458	HIS	-	expression tag	UNP Q6NCB2
C	459	HIS	-	expression tag	UNP Q6NCB2
D	7	MSE	-	initiating methionine	UNP Q6NCB2
D	452	LEU	-	expression tag	UNP Q6NCB2
D	453	GLU	-	expression tag	UNP Q6NCB2
D	454	HIS	-	expression tag	UNP Q6NCB2
D	455	HIS	-	expression tag	UNP Q6NCB2
D	456	HIS	-	expression tag	UNP Q6NCB2
D	457	HIS	-	expression tag	UNP Q6NCB2
D	458	HIS	-	expression tag	UNP Q6NCB2
D	459	HIS	-	expression tag	UNP Q6NCB2

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

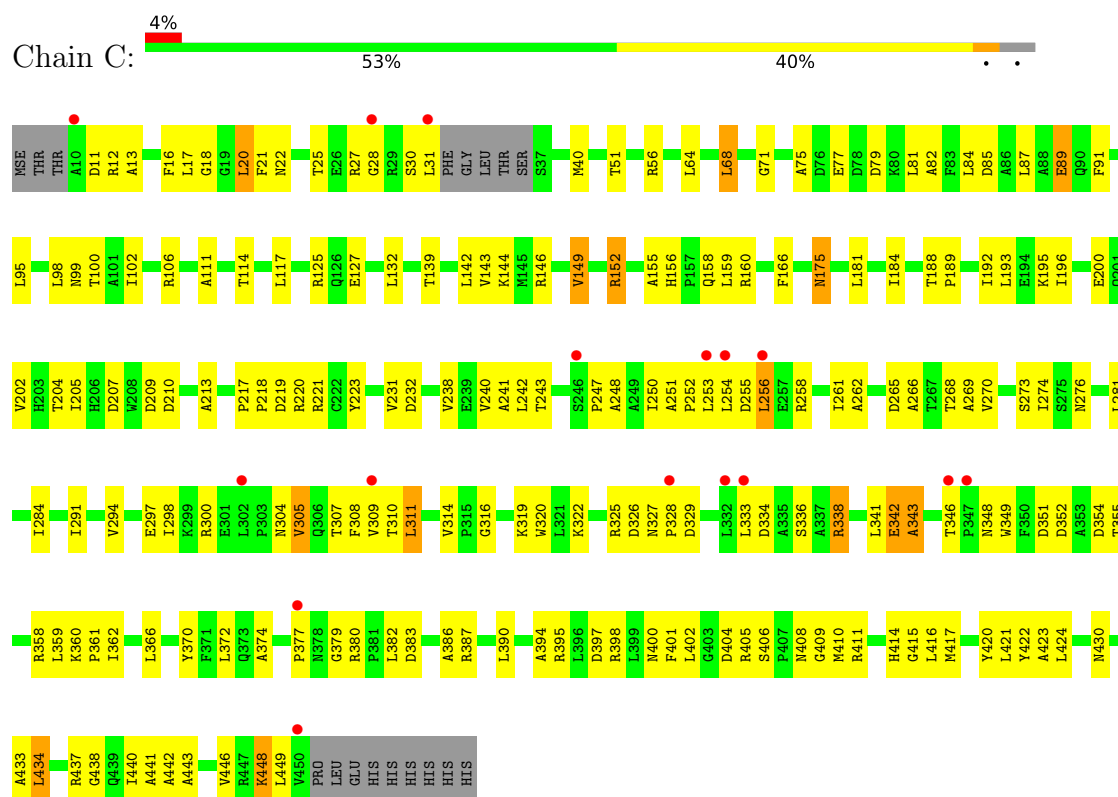
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is water.

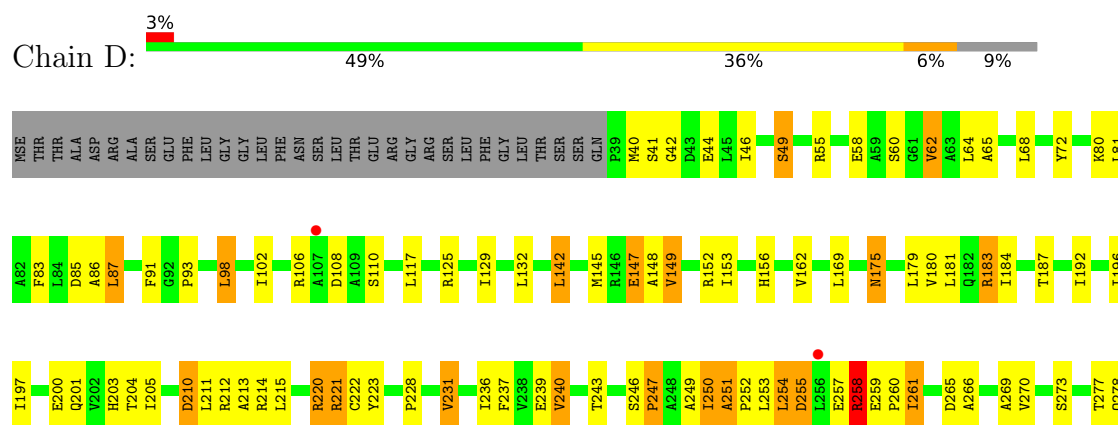
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	54	Total O 54 54	0	0
3	B	40	Total O 40 40	0	0
3	C	58	Total O 58 58	0	0
3	D	55	Total O 55 55	0	0



• Molecule 1: Malonyl-CoA decarboxylase



• Molecule 1: Malonyl-CoA decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.50Å 159.76Å 108.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.70 29.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.89-2.70) 94.8 (29.89-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.68Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.225 , 0.279 0.232 , 0.286	Depositor DCC
R_{free} test set	12810 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.0	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	0.93	EDS
Total number of atoms	13442	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	0/3472	0.97	10/4711 (0.2%)
1	B	0.46	0/3273	0.96	7/4443 (0.2%)
1	C	0.47	0/3464	0.91	6/4698 (0.1%)
1	D	0.47	0/3288	0.97	14/4465 (0.3%)
All	All	0.48	0/13497	0.95	37/18317 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	THR	N-CA-C	13.90	126.51	111.36
1	D	277	THR	N-CA-C	10.14	124.17	111.69
1	A	162	VAL	N-CA-C	-7.41	103.72	111.58
1	D	91	PHE	N-CA-C	7.38	120.91	112.57
1	A	420	TYR	N-CA-C	-6.99	98.83	109.95
1	D	201	GLN	N-CA-C	6.92	121.81	112.88
1	D	210	ASP	N-CA-C	-6.62	104.07	111.28
1	C	397	ASP	N-CA-C	6.61	119.46	111.40
1	A	270	VAL	N-CA-C	6.59	117.76	107.28
1	B	173	TRP	N-CA-C	6.33	118.18	111.28
1	A	15	GLU	N-CA-C	-6.27	104.13	110.97
1	A	277	THR	N-CA-C	6.23	120.62	112.89
1	D	326	ASP	N-CA-C	-6.14	103.14	111.55
1	D	314	VAL	CA-C-N	6.08	127.44	119.84
1	D	314	VAL	C-N-CA	6.08	127.44	119.84
1	B	323	ARG	N-CA-C	-5.98	106.14	113.50
1	C	276	ASN	N-CA-C	-5.92	99.64	109.46
1	C	320	TRP	N-CA-C	-5.87	106.25	113.41
1	C	343	ALA	N-CA-C	-5.86	105.63	112.89
1	A	397	ASP	N-CA-C	5.83	120.53	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	PHE	N-CA-C	-5.74	104.94	111.14
1	D	147	GLU	N-CA-C	-5.69	105.08	111.28
1	A	135	ALA	CA-C-N	-5.65	113.94	119.76
1	A	135	ALA	C-N-CA	-5.65	113.94	119.76
1	C	231	VAL	N-CA-C	5.52	116.82	109.37
1	B	328	PRO	N-CA-C	-5.52	106.34	113.57
1	D	312	SER	N-CA-C	5.48	118.83	110.50
1	B	358	ARG	N-CA-C	-5.34	106.93	113.50
1	D	396	LEU	N-CA-C	-5.24	101.60	109.15
1	A	275	SER	N-CA-C	5.20	117.93	109.24
1	A	243	THR	N-CA-C	5.12	115.81	108.74
1	B	270	VAL	N-CA-C	5.11	115.40	107.28
1	C	82	ALA	N-CA-C	-5.05	105.77	111.28
1	D	342	GLU	N-CA-C	-5.03	107.69	113.88
1	D	243	THR	N-CA-C	5.03	114.93	108.34
1	D	390	LEU	N-CA-C	-5.02	105.81	111.28
1	D	49	SER	N-CA-C	-5.00	105.52	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3405	0	3369	147	0
1	B	3208	0	3180	184	0
1	C	3398	0	3364	153	0
1	D	3222	0	3196	166	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	54	0	0	5	0
3	B	40	0	0	0	0
3	C	58	0	0	1	0
3	D	55	0	0	1	0
All	All	13442	0	13109	638	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 24.

All (638) 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:A:8:THR:HG22	1:A:12:ARG:HB2	1.43	0.98
1:B:318:ALA:HB2	1:B:412:GLN:HA	1.43	0.98
1:A:380:ARG:HH11	1:A:380:ARG:HB3	1.26	0.98
1:A:56:ARG:HB2	1:A:56:ARG:HH21	1.31	0.96
1:C:256:LEU:HD23	1:C:256:LEU:H	1.34	0.93
1:B:398:ARG:HE	1:B:400:ASN:ND2	1.67	0.93
1:D:424:LEU:HD12	1:D:424:LEU:H	1.37	0.89
1:B:98:LEU:O	1:B:102:ILE:HG13	1.73	0.88
1:D:175:ASN:H	1:D:175:ASN:HD22	1.21	0.88
1:C:311:LEU:HD22	1:C:417:MSE:HE2	1.54	0.88
1:C:248:ALA:HA	1:C:400:ASN:ND2	1.88	0.88
1:A:145:MSE:HE2	1:A:166:PHE:HZ	1.39	0.87
1:B:248:ALA:HB1	1:B:400:ASN:HB3	1.56	0.87
1:C:102:ILE:HD11	1:D:117:LEU:HD21	1.55	0.86
1:C:248:ALA:HB2	1:C:398:ARG:HH22	1.39	0.85
1:C:261:ILE:HD12	1:C:265:ASP:O	1.78	0.84
1:B:248:ALA:CB	1:B:400:ASN:HD22	1.91	0.83
1:B:319:LYS:H	1:B:319:LYS:HD2	1.45	0.82
1:A:102:ILE:HD11	1:B:117:LEU:HD21	1.62	0.81
1:B:279:GLN:HE21	1:B:279:GLN:HA	1.45	0.80
1:D:251:ALA:HB3	1:D:252:PRO:HD3	1.64	0.79
1:B:250:ILE:HD12	1:B:251:ALA:N	1.98	0.79
1:A:332:LEU:HD22	1:A:451:PRO:HG3	1.64	0.78
1:B:183:ARG:HH21	1:B:183:ARG:HG3	1.48	0.78
1:D:250:ILE:HD11	1:D:404:ASP:HA	1.65	0.78
1:B:398:ARG:HE	1:B:400:ASN:HD21	1.32	0.78
1:C:16:PHE:CE2	1:D:231:VAL:HA	2.19	0.77
1:D:318:ALA:O	1:D:322:LYS:HD3	1.85	0.77
1:B:268:THR:HG22	1:B:307:THR:CG2	2.16	0.76
1:A:268:THR:HG23	1:A:307:THR:OG1	1.87	0.75
1:D:183:ARG:HG2	1:D:183:ARG:HH21	1.50	0.75
1:D:325:ARG:HD3	1:D:341:LEU:HD23	1.68	0.75
1:B:398:ARG:HG3	1:B:398:ARG:HH11	1.49	0.75
1:A:358:ARG:HG2	1:A:358:ARG:HH11	1.49	0.74
1:B:106:ARG:HG2	1:B:106:ARG:HH21	1.49	0.74
1:C:311:LEU:HD22	1:C:417:MSE:CE	2.18	0.73
1:A:250:ILE:HG23	1:A:311:LEU:HD13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:HIS:HD1	1:A:229:ARG:H	1.36	0.72
1:D:98:LEU:O	1:D:102:ILE:HG13	1.89	0.72
1:A:250:ILE:HD12	1:A:251:ALA:H	1.54	0.72
1:C:404:ASP:OD2	1:C:409:GLY:HA3	1.88	0.72
1:B:248:ALA:HB2	1:B:400:ASN:HD22	1.53	0.72
1:B:404:ASP:HB2	1:B:417:MSE:HE3	1.70	0.72
1:B:343:ALA:HB3	1:B:359:LEU:HD21	1.70	0.71
1:D:58:GLU:O	1:D:62:VAL:HG12	1.90	0.71
1:D:200:GLU:HG3	1:D:205:ILE:HD11	1.71	0.71
1:C:84:LEU:HD22	1:C:149:VAL:HG12	1.73	0.70
1:C:355:THR:HA	1:C:358:ARG:HD3	1.71	0.70
1:C:175:ASN:HD22	1:C:175:ASN:H	1.40	0.70
1:B:358:ARG:HD3	1:B:359:LEU:HG	1.72	0.70
1:D:147:GLU:HG2	1:D:279:GLN:HB2	1.74	0.70
1:A:239:GLU:HB2	1:A:273:SER:HB3	1.74	0.69
1:A:181:LEU:HD11	1:A:223:TYR:HB3	1.75	0.69
1:C:21:PHE:O	1:C:25:THR:HG23	1.92	0.69
1:C:152:ARG:HB3	1:C:159:LEU:HD12	1.74	0.69
1:D:424:LEU:HD12	1:D:424:LEU:N	2.07	0.69
1:A:145:MSE:HE2	1:A:166:PHE:CZ	2.25	0.69
1:A:42:GLY:O	1:A:46:ILE:HG13	1.94	0.68
1:D:72:TYR:CE2	1:D:80:LYS:HG2	2.29	0.67
1:B:184:ILE:O	1:B:215:LEU:HD22	1.95	0.67
1:C:248:ALA:CB	1:C:398:ARG:HH22	2.05	0.67
1:D:200:GLU:HG3	1:D:205:ILE:CD1	2.24	0.67
1:B:344:LEU:HD23	1:B:359:LEU:HD13	1.76	0.67
1:B:448:LYS:HG3	1:B:449:LEU:HD12	1.77	0.67
1:A:175:ASN:N	1:A:175:ASN:HD22	1.93	0.67
1:C:27:ARG:O	1:C:30:SER:HB3	1.93	0.67
1:B:210:ASP:O	1:B:213:ALA:HB3	1.94	0.67
1:B:398:ARG:NE	1:B:400:ASN:ND2	2.41	0.67
1:C:160:ARG:O	1:C:160:ARG:HD3	1.95	0.67
1:A:221:ARG:HG2	1:A:221:ARG:HH11	1.58	0.66
1:B:68:LEU:HD13	1:B:132:LEU:HD21	1.76	0.66
1:B:370:TYR:O	1:B:374:ALA:HB3	1.95	0.66
1:C:266:ALA:O	1:C:304:ASN:ND2	2.27	0.66
1:D:424:LEU:H	1:D:424:LEU:CD1	2.07	0.66
1:D:371:PHE:CE1	1:D:418:VAL:HG11	2.30	0.66
1:C:448:LYS:C	1:C:449:LEU:HD12	2.21	0.66
1:C:360:LYS:HG2	1:C:401:PHE:CD2	2.31	0.65
1:D:394:ALA:HB2	1:D:422:TYR:CZ	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ALA:O	1:B:427:ILE:HG13	1.96	0.65
1:C:270:VAL:HA	1:C:309:VAL:O	1.97	0.64
1:C:370:TYR:O	1:C:374:ALA:HB3	1.97	0.64
1:A:315:PRO:HA	1:A:412:GLN:HG2	1.78	0.64
1:C:95:LEU:H	1:C:95:LEU:HD22	1.60	0.64
1:D:340:ALA:O	1:D:359:LEU:HD21	1.98	0.64
1:A:216:ALA:N	1:A:217:PRO:HD2	2.12	0.64
1:B:268:THR:HG22	1:B:307:THR:HG21	1.80	0.64
1:D:339:THR:HG23	1:D:340:ALA:H	1.62	0.64
1:B:260:PRO:C	1:B:261:ILE:HD12	2.23	0.63
1:C:181:LEU:HD11	1:C:223:TYR:HB3	1.79	0.63
1:B:106:ARG:HG2	1:B:106:ARG:NH2	2.12	0.63
1:D:402:LEU:CD2	1:D:410:MSE:HE1	2.28	0.63
1:B:268:THR:HG22	1:B:307:THR:HG23	1.78	0.63
1:C:114:THR:OG1	1:D:93:PRO:HG3	1.99	0.63
1:D:322:LYS:HE3	1:D:414:HIS:CE1	2.34	0.63
1:B:371:PHE:CE1	1:B:418:VAL:HG11	2.34	0.63
1:B:360:LYS:HG2	1:B:401:PHE:CD2	2.33	0.62
1:C:111:ALA:HA	1:C:114:THR:HG22	1.81	0.62
1:D:106:ARG:HH21	1:D:106:ARG:HG2	1.62	0.62
1:D:278:GLN:HB2	1:D:281:LEU:HB2	1.80	0.62
1:D:183:ARG:HG2	1:D:183:ARG:NH2	2.11	0.62
1:B:200:GLU:HG3	1:B:205:ILE:HG13	1.81	0.62
1:C:175:ASN:HD22	1:C:175:ASN:N	1.97	0.62
1:B:349:TRP:CH2	1:B:402:LEU:HD11	2.35	0.62
1:A:368:ALA:HB1	1:A:450:VAL:HG12	1.82	0.62
1:C:68:LEU:HD13	1:C:132:LEU:HD21	1.82	0.62
1:C:256:LEU:H	1:C:256:LEU:CD2	2.10	0.62
1:D:175:ASN:H	1:D:175:ASN:ND2	1.95	0.62
1:B:221:ARG:HH11	1:B:221:ARG:HG3	1.65	0.62
1:D:350:PHE:HB2	1:D:405:ARG:NH1	2.13	0.62
1:C:12:ARG:HG2	1:C:12:ARG:HH21	1.64	0.62
1:B:220:ARG:NH1	1:B:258:ARG:HH12	1.97	0.62
1:D:334:ASP:H	1:D:337:ALA:HB2	1.64	0.62
1:B:341:LEU:HD13	1:B:341:LEU:O	2.00	0.61
1:B:146:ARG:HH11	1:B:284:ILE:CD1	2.12	0.61
1:D:210:ASP:O	1:D:213:ALA:HB3	2.00	0.61
1:C:322:LYS:HE3	1:C:326:ASP:OD1	2.00	0.61
1:D:424:LEU:HA	1:D:427:ILE:HD12	1.81	0.61
1:D:301:GLU:HG2	1:D:302:LEU:HG	1.82	0.60
1:B:146:ARG:HH11	1:B:284:ILE:HD11	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HH21	1:A:56:ARG:CB	2.07	0.60
1:A:145:MSE:CE	1:A:166:PHE:HZ	2.11	0.60
1:A:102:ILE:HD13	1:A:117:LEU:HD21	1.82	0.60
1:B:279:GLN:HA	1:B:279:GLN:NE2	2.15	0.60
1:C:85:ASP:O	1:C:89:GLU:HG2	2.02	0.60
1:D:325:ARG:NH2	1:D:341:LEU:HB3	2.17	0.60
1:B:263:ALA:HB1	1:B:302:LEU:CD2	2.32	0.59
1:D:239:GLU:HB2	1:D:273:SER:HB3	1.82	0.59
1:C:51:THR:HG22	1:C:64:LEU:HD13	1.84	0.59
1:C:382:LEU:HD23	1:C:382:LEU:O	2.02	0.59
1:D:327:ASN:HB3	1:D:338:ARG:NH2	2.18	0.59
1:A:202:VAL:HG21	1:A:272:TYR:HE1	1.67	0.59
1:A:205:ILE:HG23	1:A:210:ASP:HB2	1.83	0.59
1:B:202:VAL:HG21	1:B:274:ILE:H	1.66	0.59
1:B:349:TRP:CZ3	1:B:402:LEU:HD11	2.38	0.59
1:A:175:ASN:HD22	1:A:175:ASN:H	1.50	0.59
1:B:90:GLN:O	1:B:124:ARG:NH1	2.35	0.59
1:D:197:ILE:HD11	1:D:211:LEU:HD22	1.84	0.59
1:A:325:ARG:HD3	1:A:341:LEU:HD23	1.85	0.59
1:B:309:VAL:HG22	1:B:310:THR:N	2.17	0.59
1:B:220:ARG:NH1	1:B:258:ARG:NH1	2.51	0.58
1:B:321:LEU:HA	1:B:324:GLU:HB2	1.85	0.58
1:A:93:PRO:HG3	1:B:114:THR:HG21	1.85	0.58
1:B:344:LEU:CD2	1:B:359:LEU:HD13	2.34	0.58
1:C:408:ASN:HA	1:C:411:ARG:NH1	2.17	0.58
1:D:250:ILE:HD12	1:D:251:ALA:H	1.68	0.58
1:B:375:LYS:HG3	1:B:380:ARG:O	2.03	0.58
1:A:94:ASP:OD2	1:A:94:ASP:C	2.46	0.58
1:B:278:GLN:HB2	1:B:281:LEU:HB2	1.85	0.58
1:B:297:GLU:HA	1:B:300:ARG:HG2	1.85	0.58
1:B:341:LEU:HD23	1:B:362:ILE:HD13	1.85	0.58
1:A:300:ARG:HG3	1:A:300:ARG:HH11	1.69	0.58
1:A:443:ALA:O	1:A:446:VAL:HG12	2.04	0.58
1:A:250:ILE:HD12	1:A:251:ALA:N	2.18	0.58
1:A:380:ARG:HB3	1:A:380:ARG:NH1	2.09	0.57
1:C:273:SER:C	1:C:274:ILE:HD12	2.30	0.57
1:D:212:ARG:HG2	1:D:212:ARG:HH11	1.68	0.57
1:B:149:VAL:HG23	1:B:150:LEU:N	2.19	0.57
1:B:181:LEU:HD11	1:B:223:TYR:HB3	1.86	0.57
1:B:348:ASN:HB3	1:B:351:ASP:OD2	2.04	0.57
1:C:91:PHE:O	1:C:125:ARG:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ILE:O	1:D:253:LEU:N	2.37	0.57
1:D:68:LEU:O	1:D:68:LEU:HD23	2.04	0.57
1:D:106:ARG:HG2	1:D:106:ARG:NH2	2.17	0.57
1:B:175:ASN:H	1:B:175:ASN:HD22	1.51	0.57
1:C:12:ARG:HG2	1:C:12:ARG:NH2	2.19	0.57
1:C:87:LEU:O	1:C:125:ARG:HD3	2.05	0.57
1:D:430:ASN:HB3	3:D:503:HOH:O	2.04	0.57
1:B:152:ARG:HG2	1:B:152:ARG:HH21	1.70	0.57
1:B:408:ASN:O	1:B:411:ARG:HB2	2.05	0.57
1:C:248:ALA:HB2	1:C:398:ARG:NH2	2.17	0.57
1:C:98:LEU:O	1:C:102:ILE:HG12	2.05	0.57
1:A:241:ALA:HB3	1:A:270:VAL:HG13	1.85	0.57
1:C:346:THR:OG1	1:C:349:TRP:HB3	2.05	0.56
1:D:81:LEU:HD11	1:D:156:HIS:CD2	2.39	0.56
1:D:181:LEU:HD11	1:D:223:TYR:HB3	1.87	0.56
1:D:371:PHE:HE1	1:D:418:VAL:HG11	1.69	0.56
1:B:413:SER:OG	1:B:416:LEU:HB3	2.04	0.56
1:D:330:SER:HB2	1:D:332:LEU:HD13	1.87	0.56
1:A:328:PRO:HG2	1:A:329:ASP:OD1	2.06	0.56
1:B:358:ARG:H	1:B:358:ARG:HD2	1.71	0.56
1:C:421:LEU:HD23	1:C:421:LEU:C	2.30	0.56
1:D:203:HIS:NE2	1:D:250:ILE:HG21	2.20	0.56
1:D:125:ARG:O	1:D:129:ILE:HG12	2.05	0.56
1:D:221:ARG:CB	1:D:240:VAL:HG22	2.36	0.56
1:B:302:LEU:C	1:B:304:ASN:H	2.12	0.55
1:A:144:LYS:NZ	3:A:621:HOH:O	2.39	0.55
1:B:245:ASP:OD1	1:B:247:PRO:HD3	2.06	0.55
1:C:251:ALA:N	1:C:252:PRO:HD2	2.20	0.55
1:A:288:ASN:O	1:A:392:ASN:HA	2.07	0.55
1:D:214:ARG:O	1:D:220:ARG:HG2	2.06	0.55
1:D:292:LYS:HE2	1:D:296:GLU:OE1	2.06	0.55
1:D:340:ALA:C	1:D:359:LEU:HD21	2.30	0.55
1:A:315:PRO:HA	1:A:412:GLN:CG	2.36	0.55
1:B:247:PRO:HG2	1:B:311:LEU:HD12	1.88	0.55
1:D:350:PHE:HB2	1:D:405:ARG:HH12	1.71	0.55
1:C:28:GLY:C	1:C:30:SER:H	2.15	0.54
1:D:332:LEU:HD12	1:D:332:LEU:N	2.22	0.54
1:D:333:LEU:HD22	1:D:337:ALA:HB1	1.89	0.54
1:C:448:LYS:NZ	1:C:448:LYS:HB3	2.22	0.54
1:D:65:ALA:HB1	1:D:132:LEU:HA	1.90	0.54
1:D:402:LEU:HA	1:D:415:GLY:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ALA:C	1:A:425:GLY:H	2.15	0.54
1:B:183:ARG:HG3	1:B:183:ARG:NH2	2.20	0.54
1:A:405:ARG:HA	1:A:410:MSE:HE2	1.90	0.54
1:A:432:GLU:O	1:A:436:GLU:HB2	2.08	0.54
1:A:423:ALA:HB3	1:A:426:ASP:OD2	2.07	0.54
1:C:446:VAL:O	1:C:449:LEU:HD13	2.08	0.54
1:D:319:LYS:O	1:D:323:ARG:HG3	2.07	0.54
1:A:58:GLU:O	1:A:62:VAL:HG23	2.07	0.53
1:B:197:ILE:HG22	1:B:198:ARG:N	2.23	0.53
1:D:444:SER:C	1:D:446:VAL:H	2.14	0.53
1:A:404:ASP:O	1:A:415:GLY:HA2	2.09	0.53
1:B:84:LEU:HD13	1:B:149:VAL:HG12	1.91	0.53
1:B:318:ALA:HB2	1:B:412:GLN:CA	2.29	0.53
1:C:404:ASP:HB2	1:C:417:MSE:SE	2.58	0.53
1:A:127:GLU:O	1:A:131:ARG:HG3	2.08	0.53
1:D:221:ARG:HH21	1:D:301:GLU:CD	2.16	0.53
1:A:102:ILE:CD1	1:A:117:LEU:HD21	2.38	0.53
1:B:79:ASP:O	1:B:82:ALA:HB3	2.08	0.53
1:B:398:ARG:HG3	1:B:398:ARG:NH1	2.21	0.53
1:B:146:ARG:HH21	1:B:150:LEU:HD21	1.73	0.53
1:B:263:ALA:HB1	1:B:302:LEU:HD22	1.91	0.53
1:B:371:PHE:CD1	1:B:396:LEU:HD21	2.44	0.53
1:C:338:ARG:O	1:C:342:GLU:HG3	2.09	0.53
1:A:22:ASN:O	1:A:26:GLU:HG2	2.09	0.53
1:A:367:ALA:O	1:A:370:TYR:HB3	2.09	0.53
1:B:338:ARG:HG3	1:B:338:ARG:HH21	1.74	0.53
1:A:202:VAL:HG23	1:A:203:HIS:H	1.74	0.52
1:D:49:SER:OG	1:D:83:PHE:HE2	1.92	0.52
1:A:380:ARG:HH11	1:A:380:ARG:CB	2.12	0.52
1:D:343:ALA:HB3	1:D:359:LEU:HD11	1.90	0.52
1:A:218:PRO:O	1:A:263:ALA:HB2	2.10	0.52
1:C:241:ALA:HB3	1:C:270:VAL:HG13	1.90	0.52
1:D:68:LEU:HD13	1:D:132:LEU:HD21	1.91	0.52
1:D:317:PHE:HB3	1:D:413:SER:CB	2.38	0.52
1:C:221:ARG:HH11	1:C:221:ARG:HG2	1.75	0.52
1:D:247:PRO:HG3	1:D:270:VAL:HG11	1.91	0.52
1:D:370:TYR:CE2	1:D:383:ASP:HB2	2.44	0.52
1:A:156:HIS:HB3	1:A:158:GLN:OE1	2.09	0.52
1:A:254:LEU:O	1:A:256:LEU:HD22	2.10	0.52
1:A:444:SER:O	1:A:448:LYS:HG2	2.10	0.52
1:D:46:ILE:HD11	1:D:86:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASN:HD22	1:D:175:ASN:N	1.99	0.52
1:D:394:ALA:HB2	1:D:422:TYR:CE2	2.44	0.52
1:D:398:ARG:HG3	1:D:399:LEU:N	2.25	0.52
1:B:203:HIS:CE1	1:B:250:ILE:HG21	2.44	0.52
1:B:239:GLU:HB2	1:B:273:SER:HB3	1.91	0.52
1:B:390:LEU:HD13	1:B:440:ILE:HG23	1.92	0.52
1:C:152:ARG:O	1:C:152:ARG:HD3	2.09	0.52
1:B:317:PHE:HB3	1:B:413:SER:HA	1.92	0.52
1:D:68:LEU:HD23	1:D:68:LEU:C	2.35	0.52
1:D:149:VAL:O	1:D:153:ILE:HG13	2.10	0.52
1:D:322:LYS:HE3	1:D:414:HIS:NE2	2.25	0.52
1:A:202:VAL:HG21	1:A:272:TYR:CE1	2.45	0.51
1:C:188:THR:HG23	1:C:189:PRO:HD2	1.92	0.51
1:A:381:PRO:O	1:A:387:ARG:NH1	2.43	0.51
1:B:248:ALA:HA	1:B:400:ASN:ND2	2.25	0.51
1:B:371:PHE:HE1	1:B:418:VAL:HG11	1.76	0.51
1:C:255:ASP:O	1:C:258:ARG:HD2	2.10	0.51
1:D:250:ILE:O	1:D:251:ALA:C	2.52	0.51
1:D:337:ALA:C	1:D:339:THR:H	2.18	0.51
1:B:358:ARG:CD	1:B:359:LEU:HG	2.39	0.51
1:C:401:PHE:CE2	1:C:402:LEU:HG	2.46	0.51
1:A:189:PRO:HB3	1:D:187:THR:O	2.11	0.51
1:C:20:LEU:HD13	1:D:180:VAL:HG21	1.92	0.51
1:D:395:ARG:NH2	1:D:397:ASP:OD1	2.43	0.51
1:B:139:THR:O	1:B:143:VAL:HG23	2.11	0.51
1:A:422:TYR:HD2	1:A:427:ILE:HD11	1.76	0.51
1:B:404:ASP:O	1:B:415:GLY:HA2	2.11	0.51
1:A:8:THR:CG2	1:A:12:ARG:HB2	2.27	0.51
1:A:186:TRP:CH2	1:A:212:ARG:HB2	2.45	0.51
1:C:284:ILE:HD12	1:C:284:ILE:N	2.26	0.51
1:D:147:GLU:HG3	1:D:280:GLY:N	2.26	0.51
1:C:309:VAL:HG22	1:C:310:THR:N	2.26	0.51
1:D:221:ARG:HB3	1:D:240:VAL:HG22	1.91	0.51
1:B:332:LEU:N	1:B:332:LEU:HD22	2.26	0.50
1:D:184:ILE:O	1:D:222:CYS:HB3	2.11	0.50
1:B:334:ASP:O	1:B:338:ARG:HG2	2.10	0.50
1:C:325:ARG:HD3	1:C:342:GLU:HG2	1.93	0.50
1:D:346:THR:OG1	1:D:349:TRP:HB3	2.11	0.50
1:D:403:GLY:N	1:D:415:GLY:O	2.44	0.50
1:A:89:GLU:HG3	1:A:90:GLN:HG3	1.93	0.50
1:A:220:ARG:O	1:A:221:ARG:HG2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LYS:N	3:A:610:HOH:O	2.34	0.50
1:C:77:GLU:O	1:C:81:LEU:HG	2.11	0.50
1:D:310:THR:HG21	1:D:389:HIS:CE1	2.47	0.50
1:A:375:LYS:HD2	1:A:379:GLY:O	2.12	0.50
1:C:152:ARG:HD2	1:C:156:HIS:HB2	1.94	0.50
1:D:327:ASN:OD1	1:D:330:SER:N	2.45	0.50
1:B:413:SER:O	1:B:416:LEU:HB3	2.11	0.50
1:C:81:LEU:HB3	1:C:152:ARG:HH22	1.77	0.50
1:A:186:TRP:CE2	1:A:212:ARG:HD3	2.46	0.50
1:A:214:ARG:HD3	1:A:214:ARG:C	2.37	0.50
1:B:155:ALA:C	1:B:156:HIS:ND1	2.69	0.50
1:D:330:SER:C	1:D:332:LEU:H	2.19	0.50
1:B:354:ASP:O	1:B:356:ALA:N	2.44	0.50
1:B:355:THR:HA	1:B:358:ARG:HE	1.77	0.50
1:C:443:ALA:O	1:C:446:VAL:HG12	2.12	0.50
1:D:250:ILE:CD1	1:D:251:ALA:H	2.25	0.50
1:A:302:LEU:HB3	1:A:304:ASN:OD1	2.12	0.49
1:B:216:ALA:HB3	1:B:217:PRO:HD3	1.94	0.49
1:C:380:ARG:NH1	1:C:387:ARG:HD3	2.27	0.49
1:A:47:ALA:O	1:A:50:GLU:HB2	2.13	0.49
1:B:317:PHE:HE1	1:B:367:ALA:HA	1.77	0.49
1:B:302:LEU:HB3	1:B:304:ASN:OD1	2.12	0.49
1:C:81:LEU:HB3	1:C:152:ARG:NH2	2.27	0.49
1:C:334:ASP:OD1	1:C:336:SER:HB2	2.12	0.49
1:D:373:GLN:O	1:D:375:LYS:HG2	2.11	0.49
1:A:142:LEU:HD12	1:A:166:PHE:HE1	1.76	0.49
1:A:186:TRP:CZ2	1:A:212:ARG:HD3	2.47	0.49
1:C:111:ALA:HA	1:C:114:THR:CG2	2.42	0.49
1:C:207:ASP:OD1	1:C:209:ASP:HB2	2.12	0.49
1:D:448:LYS:NZ	1:D:448:LYS:HB3	2.27	0.49
1:D:311:LEU:HD13	1:D:419:ASN:HD21	1.77	0.49
1:B:127:GLU:O	1:B:131:ARG:HG3	2.12	0.48
1:A:423:ALA:O	1:A:425:GLY:N	2.40	0.48
1:B:315:PRO:HA	1:B:412:GLN:HB3	1.94	0.48
1:C:382:LEU:HD23	1:C:382:LEU:C	2.38	0.48
1:C:410:MSE:O	1:C:414:HIS:HA	2.12	0.48
1:C:200:GLU:HG2	1:C:205:ILE:HD12	1.95	0.48
1:D:261:ILE:HG13	1:D:265:ASP:HB2	1.96	0.48
1:A:22:ASN:N	1:A:22:ASN:HD22	2.10	0.48
1:A:250:ILE:O	1:A:251:ALA:C	2.56	0.48
1:B:221:ARG:HG3	1:B:221:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ARG:HH11	1:B:398:ARG:CG	2.24	0.48
1:C:152:ARG:HB3	1:C:159:LEU:CD1	2.42	0.48
1:D:402:LEU:HD22	1:D:410:MSE:HE1	1.95	0.48
1:B:264:SER:HA	1:B:304:ASN:ND2	2.29	0.48
1:B:146:ARG:NH1	1:B:282:ALA:O	2.47	0.48
1:B:369:ALA:O	1:B:373:GLN:HB2	2.13	0.48
1:C:102:ILE:HD12	1:D:102:ILE:HG23	1.96	0.48
1:D:254:LEU:O	1:D:255:ASP:C	2.56	0.48
1:D:258:ARG:HG2	1:D:259:GLU:N	2.27	0.48
1:D:288:ASN:O	1:D:392:ASN:HA	2.13	0.48
1:B:197:ILE:HG13	1:B:211:LEU:HD22	1.95	0.48
1:C:372:LEU:HD21	1:C:442:ALA:HB3	1.96	0.48
1:D:315:PRO:HG2	1:D:384:PRO:HG2	1.94	0.48
1:D:331:THR:HG22	1:D:331:THR:O	2.13	0.48
1:D:335:ALA:C	1:D:337:ALA:H	2.21	0.48
1:B:146:ARG:NH2	1:B:163:ASP:OD1	2.47	0.48
1:B:152:ARG:HG2	1:B:152:ARG:NH2	2.27	0.48
1:B:447:ARG:HG2	1:B:447:ARG:HH11	1.79	0.48
1:C:274:ILE:HD12	1:C:274:ILE:N	2.29	0.48
1:D:284:ILE:N	1:D:284:ILE:HD12	2.29	0.48
1:C:394:ALA:HB2	1:C:422:TYR:CZ	2.48	0.48
1:C:404:ASP:O	1:C:415:GLY:HA2	2.14	0.48
1:D:196:ILE:HG23	1:D:237:PHE:CZ	2.49	0.48
1:D:249:ALA:HA	1:D:403:GLY:O	2.14	0.48
1:A:98:LEU:HA	1:A:120:ALA:HB1	1.95	0.47
1:B:146:ARG:NH1	1:B:284:ILE:CD1	2.76	0.47
1:B:371:PHE:HD1	1:B:396:LEU:HD21	1.78	0.47
1:B:261:ILE:HD12	1:B:261:ILE:N	2.29	0.47
1:A:358:ARG:HG2	1:A:358:ARG:NH1	2.22	0.47
1:C:75:ALA:HB1	1:C:79:ASP:HB2	1.96	0.47
1:D:324:GLU:OE2	1:D:332:LEU:HD22	2.14	0.47
1:D:337:ALA:C	1:D:339:THR:N	2.69	0.47
1:D:346:THR:HB	1:D:347:PRO:HD2	1.96	0.47
1:A:16:PHE:CE2	1:B:231:VAL:HA	2.50	0.47
1:D:250:ILE:HD12	1:D:250:ILE:H	1.80	0.47
1:B:200:GLU:OE2	1:B:201:GLN:N	2.47	0.47
1:D:250:ILE:HD12	1:D:250:ILE:N	2.29	0.47
1:A:147:GLU:HG3	1:A:279:GLN:HB3	1.96	0.47
1:C:111:ALA:CA	1:C:114:THR:HG22	2.45	0.47
1:C:205:ILE:HA	1:C:210:ASP:HB3	1.96	0.47
1:C:316:GLY:HA2	1:C:319:LYS:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:LYS:HB3	1:C:448:LYS:HZ3	1.80	0.47
1:D:223:TYR:CE2	1:D:297:GLU:HG2	2.50	0.47
1:D:324:GLU:O	1:D:324:GLU:HG3	2.15	0.47
1:A:18:GLY:O	1:A:22:ASN:ND2	2.47	0.47
1:A:300:ARG:HG3	1:A:300:ARG:NH1	2.30	0.47
1:A:382:LEU:O	1:A:382:LEU:HD23	2.15	0.47
1:C:31:LEU:O	1:C:31:LEU:HD23	2.15	0.47
1:C:218:PRO:HA	3:C:655:HOH:O	2.15	0.47
1:C:360:LYS:HG2	1:C:401:PHE:CE2	2.50	0.47
1:A:352:ASP:O	1:A:353:ALA:C	2.58	0.47
1:A:365:GLN:HG3	1:A:449:LEU:O	2.15	0.47
1:B:266:ALA:O	1:B:304:ASN:ND2	2.48	0.47
1:B:324:GLU:O	1:B:327:ASN:ND2	2.48	0.47
1:B:433:ALA:HB1	1:B:439:GLN:NE2	2.29	0.47
1:C:297:GLU:OE1	1:C:300:ARG:NE	2.47	0.47
1:C:440:ILE:HG22	1:C:440:ILE:O	2.13	0.47
1:D:301:GLU:HG2	1:D:302:LEU:CD2	2.45	0.47
1:B:243:THR:O	1:B:266:ALA:HB1	2.15	0.47
1:B:339:THR:C	1:B:341:LEU:H	2.22	0.47
1:C:297:GLU:O	1:C:300:ARG:HG2	2.14	0.47
1:A:245:ASP:O	1:A:247:PRO:HD3	2.14	0.46
1:B:268:THR:HA	1:B:307:THR:HG23	1.96	0.46
1:B:324:GLU:HB3	1:B:333:LEU:HD11	1.98	0.46
1:C:20:LEU:HD12	1:D:228:PRO:HD3	1.95	0.46
1:C:95:LEU:HD22	1:C:95:LEU:N	2.29	0.46
1:D:257:GLU:HG3	1:D:258:ARG:N	2.30	0.46
1:A:402:LEU:HD13	1:A:405:ARG:NH2	2.29	0.46
1:D:338:ARG:HA	1:D:341:LEU:HB2	1.98	0.46
1:A:398:ARG:HG3	1:A:399:LEU:N	2.28	0.46
1:D:205:ILE:HG12	1:D:214:ARG:CZ	2.45	0.46
1:D:333:LEU:HD21	1:D:366:LEU:HD11	1.97	0.46
1:A:20:LEU:O	1:A:24:LEU:HG	2.16	0.46
1:A:197:ILE:HG23	1:A:205:ILE:HG22	1.98	0.46
1:A:437:ARG:HB2	1:A:439:GLN:HG3	1.96	0.46
1:B:337:ALA:C	1:B:339:THR:H	2.24	0.46
1:B:346:THR:OG1	1:B:349:TRP:HB3	2.16	0.46
1:D:444:SER:O	1:D:446:VAL:N	2.49	0.46
1:B:94:ASP:OD2	1:B:94:ASP:C	2.58	0.46
1:C:250:ILE:C	1:C:252:PRO:HD2	2.40	0.46
1:A:93:PRO:HG3	1:B:114:THR:CG2	2.45	0.46
1:C:139:THR:O	1:C:143:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HG13	1:A:417:MSE:SE	2.66	0.46
1:A:370:TYR:O	1:A:374:ALA:HB3	2.16	0.46
1:C:28:GLY:C	1:C:30:SER:N	2.73	0.46
1:D:447:ARG:O	1:D:450:VAL:HG22	2.16	0.46
1:A:175:ASN:N	1:A:175:ASN:ND2	2.64	0.46
1:B:263:ALA:HB1	1:B:302:LEU:HD21	1.98	0.46
1:D:85:ASP:C	1:D:87:LEU:N	2.74	0.46
1:A:68:LEU:C	1:A:68:LEU:HD23	2.41	0.45
1:A:240:VAL:HG12	1:A:241:ALA:N	2.30	0.45
1:C:40:MSE:HE3	1:C:71:GLY:HA3	1.98	0.45
1:D:339:THR:HG23	1:D:340:ALA:N	2.28	0.45
1:A:380:ARG:O	1:A:381:PRO:C	2.59	0.45
1:B:213:ALA:O	1:B:217:PRO:HD2	2.16	0.45
1:C:195:LYS:HE3	1:C:232:ASP:O	2.16	0.45
1:D:257:GLU:HG3	1:D:258:ARG:H	1.80	0.45
1:A:153:ILE:HD13	1:A:159:LEU:HB2	1.99	0.45
1:A:221:ARG:HG2	1:A:221:ARG:NH1	2.29	0.45
1:A:258:ARG:HG2	1:A:258:ARG:HH11	1.80	0.45
1:B:81:LEU:HB2	1:B:152:ARG:HH22	1.81	0.45
1:B:261:ILE:CG2	1:B:265:ASP:HB3	2.46	0.45
1:C:200:GLU:HG2	1:C:205:ILE:CD1	2.45	0.45
1:D:41:SER:OG	1:D:44:GLU:HG3	2.17	0.45
1:D:317:PHE:HB3	1:D:413:SER:HB3	1.98	0.45
1:A:81:LEU:O	1:A:81:LEU:HD23	2.17	0.45
1:C:240:VAL:HG12	1:C:241:ALA:N	2.31	0.45
1:C:291:ILE:HG21	1:C:422:TYR:CZ	2.51	0.45
1:D:49:SER:HG	1:D:83:PHE:HE2	1.64	0.45
1:A:391:GLY:C	1:A:393:GLY:H	2.23	0.45
1:A:397:ASP:HB2	1:A:421:LEU:HB2	1.98	0.45
1:C:434:LEU:HD23	1:C:434:LEU:O	2.17	0.45
1:D:147:GLU:CG	1:D:279:GLN:HB2	2.43	0.45
1:D:42:GLY:O	1:D:46:ILE:HG13	2.17	0.45
1:A:325:ARG:HH12	1:A:345:ASP:CG	2.23	0.45
1:B:45:LEU:HB3	1:B:83:PHE:CD2	2.52	0.45
1:C:184:ILE:HG21	1:C:196:ILE:HG13	1.98	0.45
1:C:223:TYR:CE1	1:C:297:GLU:HG2	2.52	0.45
1:D:269:ALA:HB3	1:D:308:PHE:CD1	2.51	0.45
1:B:424:LEU:HD12	1:B:424:LEU:N	2.33	0.44
1:C:359:LEU:O	1:C:362:ILE:HG22	2.17	0.44
1:D:382:LEU:O	1:D:387:ARG:NH1	2.50	0.44
1:C:294:VAL:O	1:C:298:ILE:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:HA	1:A:215:LEU:HD13	1.98	0.44
1:D:444:SER:C	1:D:446:VAL:N	2.74	0.44
1:C:248:ALA:O	1:C:400:ASN:HB3	2.16	0.44
1:D:125:ARG:HD3	1:D:162:VAL:HG22	2.00	0.44
1:A:93:PRO:HD3	1:A:123:PRO:HB3	1.98	0.44
1:A:193:LEU:O	1:A:197:ILE:HG13	2.17	0.44
1:C:175:ASN:N	1:C:175:ASN:ND2	2.65	0.44
1:C:437:ARG:HG2	1:C:437:ARG:NH2	2.32	0.44
1:A:128:LEU:O	1:A:132:LEU:HG	2.18	0.44
1:B:261:ILE:HG22	1:B:265:ASP:HB3	2.00	0.44
1:B:447:ARG:HG2	1:B:447:ARG:NH1	2.32	0.44
1:A:185:ASP:O	1:A:188:THR:HB	2.17	0.44
1:A:368:ALA:CB	1:A:450:VAL:HG12	2.46	0.44
1:B:149:VAL:O	1:B:150:LEU:C	2.59	0.44
1:B:250:ILE:HA	1:B:253:LEU:HD12	1.98	0.44
1:B:302:LEU:C	1:B:304:ASN:N	2.75	0.44
1:D:250:ILE:CD1	1:D:250:ILE:H	2.30	0.44
1:D:343:ALA:HB1	1:D:355:THR:HG1	1.83	0.44
1:D:423:ALA:O	1:D:427:ILE:HG13	2.17	0.44
1:A:175:ASN:ND2	1:A:227:HIS:NE2	2.66	0.44
1:B:398:ARG:HD2	1:B:400:ASN:N	2.33	0.44
1:C:160:ARG:HD3	1:C:160:ARG:C	2.43	0.44
1:C:281:LEU:C	1:C:284:ILE:HD13	2.43	0.44
1:D:142:LEU:HA	1:D:142:LEU:HD12	1.77	0.44
1:A:140:ALA:O	1:A:144:LYS:HE2	2.18	0.43
1:B:352:ASP:OD1	1:B:352:ASP:O	2.36	0.43
1:B:372:LEU:CD1	1:B:447:ARG:HA	2.47	0.43
1:B:378:ASN:C	1:B:380:ARG:H	2.26	0.43
1:C:268:THR:HA	1:C:307:THR:O	2.18	0.43
1:C:327:ASN:C	1:C:329:ASP:H	2.25	0.43
1:C:360:LYS:HE2	1:C:360:LYS:HB3	1.87	0.43
1:D:302:LEU:C	1:D:304:ASN:H	2.26	0.43
1:B:146:ARG:O	1:B:149:VAL:HG22	2.17	0.43
1:B:219:ASP:OD2	1:B:258:ARG:NH2	2.51	0.43
1:B:311:LEU:CD2	1:B:417:MSE:SE	3.16	0.43
1:C:17:LEU:HB3	1:C:21:PHE:CE2	2.53	0.43
1:A:205:ILE:HD13	1:A:211:LEU:HD23	2.01	0.43
1:A:369:ALA:O	1:A:373:GLN:HB2	2.18	0.43
1:B:337:ALA:C	1:B:339:THR:N	2.76	0.43
1:D:255:ASP:OD1	1:D:257:GLU:HG2	2.18	0.43
1:A:38:GLN:CG	1:A:39:PRO:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ILE:HD11	1:D:404:ASP:CA	2.42	0.43
1:A:270:VAL:HA	1:A:309:VAL:O	2.17	0.43
1:A:399:LEU:HA	1:A:418:VAL:HG12	2.00	0.43
1:B:183:ARG:NH2	1:B:183:ARG:CG	2.81	0.43
1:C:89:GLU:HG2	1:C:89:GLU:H	1.61	0.43
1:C:106:ARG:HH11	1:C:106:ARG:HG2	1.83	0.43
1:D:108:ASP:OD2	1:D:110:SER:HB3	2.19	0.43
1:B:142:LEU:HD12	1:B:142:LEU:HA	1.93	0.43
1:B:271:PHE:HE1	1:B:294:VAL:HG11	1.84	0.43
1:B:317:PHE:CE1	1:B:367:ALA:HA	2.53	0.43
1:C:349:TRP:CH2	1:C:402:LEU:HD21	2.54	0.43
1:D:55:ARG:HD2	1:D:55:ARG:HA	1.80	0.43
1:C:192:ILE:O	1:C:195:LYS:HB2	2.19	0.43
1:C:423:ALA:O	1:C:424:LEU:C	2.62	0.43
1:A:309:VAL:HG22	1:A:310:THR:N	2.34	0.43
1:A:329:ASP:O	1:A:330:SER:C	2.61	0.43
1:D:192:ILE:O	1:D:196:ILE:HD12	2.18	0.43
1:B:146:ARG:NH2	1:B:150:LEU:HD21	2.34	0.43
1:C:99:ASN:O	1:C:100:THR:C	2.62	0.43
1:D:81:LEU:HD13	1:D:152:ARG:HD3	2.01	0.43
1:D:405:ARG:HG2	1:D:405:ARG:HH11	1.83	0.43
1:A:309:VAL:CG2	1:A:419:ASN:HB3	2.49	0.43
1:B:224:GLY:HA2	1:B:237:PHE:HA	2.00	0.43
1:B:248:ALA:CB	1:B:400:ASN:ND2	2.71	0.43
1:B:251:ALA:N	1:B:252:PRO:HD2	2.34	0.43
1:B:309:VAL:CG2	1:B:310:THR:N	2.80	0.43
1:B:360:LYS:O	1:B:364:LEU:HG	2.19	0.43
1:B:399:LEU:O	1:B:400:ASN:C	2.61	0.43
1:B:77:GLU:O	1:B:80:LYS:HB2	2.19	0.42
1:B:144:LYS:O	1:B:147:GLU:HB2	2.19	0.42
1:B:220:ARG:O	1:B:221:ARG:HG3	2.18	0.42
1:C:348:ASN:HB3	1:C:351:ASP:OD2	2.18	0.42
1:C:405:ARG:HA	1:C:410:MSE:HE2	2.00	0.42
1:A:193:LEU:HD22	1:A:211:LEU:HD11	2.00	0.42
1:B:160:ARG:HH21	1:B:160:ARG:HB2	1.84	0.42
1:A:94:ASP:CG	1:A:97:GLU:HG2	2.44	0.42
1:A:197:ILE:O	1:A:197:ILE:HG22	2.19	0.42
1:B:87:LEU:HD12	1:B:87:LEU:HA	1.86	0.42
1:B:297:GLU:OE2	1:B:300:ARG:HD3	2.18	0.42
1:B:398:ARG:HD2	1:B:400:ASN:H	1.84	0.42
1:C:355:THR:HA	1:C:358:ARG:CD	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LEU:HD12	1:D:179:LEU:HA	1.89	0.42
1:A:105:PHE:CE2	1:A:114:THR:HG22	2.55	0.42
1:B:371:PHE:CZ	1:B:418:VAL:HG11	2.54	0.42
1:B:398:ARG:HD2	1:B:400:ASN:CG	2.44	0.42
1:C:370:TYR:CE2	1:C:383:ASP:HB2	2.54	0.42
1:D:236:ILE:HD11	1:D:286:PHE:HD2	1.84	0.42
1:B:332:LEU:O	1:B:366:LEU:HD21	2.20	0.42
1:B:405:ARG:HG2	1:B:405:ARG:HH21	1.83	0.42
1:C:304:ASN:O	1:C:305:VAL:C	2.61	0.42
1:C:406:SER:C	1:C:408:ASN:N	2.75	0.42
1:D:314:VAL:HG12	1:D:314:VAL:O	2.19	0.42
1:A:256:LEU:HD22	1:A:256:LEU:N	2.34	0.42
1:B:146:ARG:NH1	1:B:284:ILE:HD11	2.34	0.42
1:C:359:LEU:HA	1:C:362:ILE:HG22	2.01	0.42
1:D:212:ARG:HG2	1:D:212:ARG:NH1	2.34	0.42
1:A:146:ARG:HA	1:A:149:VAL:HG13	2.00	0.42
1:C:269:ALA:HB3	1:C:308:PHE:CD2	2.55	0.42
1:D:301:GLU:HG2	1:D:302:LEU:CG	2.46	0.42
1:A:219:ASP:CG	1:A:258:ARG:HH21	2.28	0.42
1:C:18:GLY:O	1:C:22:ASN:ND2	2.52	0.42
1:C:395:ARG:O	1:C:420:TYR:HA	2.20	0.42
1:A:118:LEU:HD22	1:B:123:PRO:HD3	2.02	0.42
1:A:219:ASP:HA	1:A:242:LEU:HD23	2.02	0.42
1:A:221:ARG:NH1	1:A:221:ARG:CG	2.82	0.42
1:B:149:VAL:CG2	1:B:150:LEU:N	2.81	0.42
1:B:223:TYR:N	1:B:223:TYR:CD1	2.88	0.42
1:B:223:TYR:CE2	1:B:297:GLU:HG2	2.55	0.42
1:B:341:LEU:HD23	1:B:362:ILE:CD1	2.49	0.42
1:B:395:ARG:NH1	1:B:421:LEU:HD23	2.35	0.42
1:C:394:ALA:HB2	1:C:422:TYR:CE2	2.55	0.42
1:A:335:ALA:HA	3:A:631:HOH:O	2.19	0.41
1:B:69:LEU:O	1:B:73:GLU:HB2	2.20	0.41
1:C:219:ASP:HA	1:C:242:LEU:HB2	2.02	0.41
1:C:247:PRO:HG3	1:C:253:LEU:HD11	2.02	0.41
1:C:354:ASP:O	1:C:358:ARG:HD3	2.20	0.41
1:D:145:MSE:O	1:D:148:ALA:HB3	2.19	0.41
1:D:266:ALA:O	1:D:304:ASN:ND2	2.49	0.41
1:D:404:ASP:HB2	1:D:417:MSE:SE	2.70	0.41
1:A:212:ARG:HG2	1:A:212:ARG:HH21	1.84	0.41
1:A:380:ARG:NH1	3:A:653:HOH:O	2.52	0.41
1:B:339:THR:C	1:B:341:LEU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:LYS:HB2	1:C:361:PRO:CD	2.50	0.41
1:C:386:ALA:O	1:C:390:LEU:HB2	2.20	0.41
1:C:430:ASN:O	1:C:433:ALA:HB3	2.20	0.41
1:D:40:MSE:HA	1:D:44:GLU:OE1	2.20	0.41
1:A:394:ALA:HB2	1:A:422:TYR:CE2	2.55	0.41
1:A:437:ARG:CB	1:A:439:GLN:HG3	2.49	0.41
1:B:338:ARG:HG3	1:B:338:ARG:NH2	2.34	0.41
1:B:347:PRO:HG2	1:B:348:ASN:H	1.86	0.41
1:B:374:ALA:O	1:B:375:LYS:HD2	2.20	0.41
1:C:146:ARG:HD2	1:C:166:PHE:HB3	2.00	0.41
1:C:219:ASP:O	1:C:220:ARG:NH2	2.52	0.41
1:C:314:VAL:HG12	1:C:314:VAL:O	2.20	0.41
1:A:155:ALA:C	1:A:156:HIS:ND1	2.79	0.41
1:C:243:THR:HA	1:C:261:ILE:HD11	2.02	0.41
1:D:334:ASP:O	1:D:337:ALA:HB3	2.20	0.41
1:D:450:VAL:O	1:D:450:VAL:HG23	2.19	0.41
1:A:125:ARG:NE	1:A:165:ASP:OD1	2.53	0.41
1:A:422:TYR:HD2	1:A:427:ILE:CD1	2.33	0.41
1:C:111:ALA:O	1:C:114:THR:HG22	2.20	0.41
1:C:250:ILE:HG13	1:C:254:LEU:HD13	2.02	0.41
1:A:144:LYS:HD3	3:A:622:HOH:O	2.20	0.41
1:C:221:ARG:HG2	1:C:221:ARG:NH1	2.35	0.41
1:D:60:SER:O	1:D:64:LEU:HG	2.21	0.41
1:B:148:ALA:O	1:B:152:ARG:HD2	2.21	0.41
1:C:362:ILE:O	1:C:366:LEU:HG	2.20	0.41
1:D:336:SER:C	1:D:339:THR:HG22	2.46	0.41
1:A:38:GLN:CD	1:A:39:PRO:HD2	2.46	0.41
1:C:40:MSE:HE3	1:C:71:GLY:CA	2.50	0.41
1:D:68:LEU:C	1:D:68:LEU:CD2	2.94	0.41
1:D:327:ASN:HA	1:D:328:PRO:HD3	1.88	0.41
1:A:406:SER:O	1:A:407:PRO:C	2.64	0.41
1:B:87:LEU:O	1:B:125:ARG:HD3	2.21	0.41
1:B:199:TYR:O	1:B:200:GLU:C	2.59	0.41
1:B:337:ALA:O	1:B:339:THR:N	2.54	0.41
1:B:355:THR:HG23	1:B:355:THR:O	2.21	0.41
1:C:11:ASP:C	1:C:13:ALA:N	2.77	0.41
1:C:155:ALA:O	1:C:156:HIS:ND1	2.54	0.41
1:C:238:VAL:O	1:C:238:VAL:HG12	2.20	0.41
1:C:341:LEU:C	1:C:343:ALA:H	2.29	0.41
1:D:147:GLU:HG2	1:D:279:GLN:CB	2.48	0.41
1:D:314:VAL:HG12	1:D:317:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:HA	1:A:260:PRO:HD2	1.89	0.41
1:A:437:ARG:NH2	1:A:437:ARG:HG2	2.36	0.41
1:B:146:ARG:NH2	1:B:150:LEU:HD11	2.36	0.41
1:B:188:THR:HG23	1:B:189:PRO:HD2	2.03	0.41
1:C:188:THR:HG22	1:C:193:LEU:HG	2.01	0.41
1:A:55:ARG:HD2	1:A:55:ARG:HA	1.87	0.40
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.95	0.40
1:C:204:THR:C	1:C:205:ILE:HG13	2.46	0.40
1:C:213:ALA:O	1:C:217:PRO:HD2	2.21	0.40
1:D:386:ALA:O	1:D:390:LEU:HB2	2.20	0.40
1:A:219:ASP:HA	1:A:242:LEU:HB2	2.03	0.40
1:B:122:GLU:HA	1:B:123:PRO:HD3	1.94	0.40
1:B:360:LYS:N	1:B:361:PRO:HD2	2.37	0.40
1:C:262:ALA:O	1:C:265:ASP:HB2	2.21	0.40
1:D:246:SER:HA	1:D:247:PRO:HD2	1.85	0.40
1:D:378:ASN:HD22	1:D:378:ASN:HA	1.58	0.40
1:D:448:LYS:NZ	1:D:448:LYS:CB	2.85	0.40
1:A:175:ASN:H	1:A:175:ASN:ND2	2.18	0.40
1:B:159:LEU:O	1:B:160:ARG:C	2.64	0.40
1:A:264:SER:O	1:A:304:ASN:ND2	2.55	0.40
1:A:359:LEU:O	1:A:362:ILE:HG22	2.20	0.40
1:B:319:LYS:H	1:B:319:LYS:CD	2.15	0.40
1:D:197:ILE:CD1	1:D:211:LEU:HD22	2.51	0.40
1:D:311:LEU:CD1	1:D:419:ASN:HD21	2.35	0.40
1:D:370:TYR:CZ	1:D:383:ASP:HB2	2.56	0.40
1:B:403:GLY:N	1:B:415:GLY:O	2.55	0.40
1:C:240:VAL:CG1	1:C:241:ALA:N	2.84	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	433/453 (96%)	388 (90%)	38 (9%)	7 (2%)	7	20
1	B	409/453 (90%)	358 (88%)	37 (9%)	14 (3%)	3	7
1	C	432/453 (95%)	374 (87%)	48 (11%)	10 (2%)	5	13
1	D	411/453 (91%)	359 (87%)	38 (9%)	14 (3%)	3	7
All	All	1685/1812 (93%)	1479 (88%)	161 (10%)	45 (3%)	4	10

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	VAL
1	B	354	ASP
1	B	355	THR
1	D	260	PRO
1	D	354	ASP
1	A	424	LEU
1	B	318	ALA
1	B	356	ALA
1	C	305	VAL
1	D	247	PRO
1	D	258	ARG
1	D	329	ASP
1	D	445	ALA
1	A	379	GLY
1	B	109	ALA
1	B	204	THR
1	B	400	ASN
1	C	202	VAL
1	C	352	ASP
1	D	348	ASN
1	A	203	HIS
1	A	445	ALA
1	B	232	ASP
1	B	245	ASP
1	B	338	ARG
1	B	425	GLY
1	C	338	ARG
1	C	342	GLU
1	C	377	PRO
1	D	356	ALA
1	A	347	PRO
1	A	353	ALA
1	B	374	ALA

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Mol	Chain	Res	Type
1	C	379	GLY
1	C	441	ALA
1	D	204	THR
1	D	255	ASP
1	B	347	PRO
1	D	261	ILE
1	D	315	PRO
1	B	247	PRO
1	D	316	GLY
1	C	438	GLY
1	D	251	ALA
1	C	328	PRO

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	350/360 (97%)	326 (93%)	24 (7%)	14	34
1	B	329/360 (91%)	304 (92%)	25 (8%)	12	30
1	C	349/360 (97%)	331 (95%)	18 (5%)	21	47
1	D	331/360 (92%)	308 (93%)	23 (7%)	14	34
All	All	1359/1440 (94%)	1269 (93%)	90 (7%)	15	36

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	56	ARG
1	A	95	LEU
1	A	117	LEU
1	A	149	VAL
1	A	158	GLN
1	A	175	ASN
1	A	176	ARG
1	A	188	THR

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Mol	Chain	Res	Type
1	A	202	VAL
1	A	221	ARG
1	A	242	LEU
1	A	250	ILE
1	A	275	SER
1	A	276	ASN
1	A	292	LYS
1	A	311	LEU
1	A	332	LEU
1	A	341	LEU
1	A	358	ARG
1	A	380	ARG
1	A	382	LEU
1	A	416	LEU
1	A	426	ASP
1	B	62	VAL
1	B	87	LEU
1	B	89	GLU
1	B	98	LEU
1	B	106	ARG
1	B	118	LEU
1	B	127	GLU
1	B	142	LEU
1	B	146	ARG
1	B	169	LEU
1	B	175	ASN
1	B	220	ARG
1	B	275	SER
1	B	279	GLN
1	B	281	LEU
1	B	295	VAL
1	B	307	THR
1	B	312	SER
1	B	341	LEU
1	B	358	ARG
1	B	382	LEU
1	B	392	ASN
1	B	398	ARG
1	B	400	ASN
1	B	426	ASP
1	C	20	LEU
1	C	56	ARG

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Mol	Chain	Res	Type
1	C	68	LEU
1	C	89	GLU
1	C	117	LEU
1	C	127	GLU
1	C	142	LEU
1	C	144	LYS
1	C	149	VAL
1	C	152	ARG
1	C	158	GLN
1	C	175	ASN
1	C	256	LEU
1	C	311	LEU
1	C	333	LEU
1	C	416	LEU
1	C	434	LEU
1	C	448	LYS
1	D	62	VAL
1	D	87	LEU
1	D	98	LEU
1	D	142	LEU
1	D	149	VAL
1	D	169	LEU
1	D	175	ASN
1	D	183	ARG
1	D	215	LEU
1	D	220	ARG
1	D	221	ARG
1	D	231	VAL
1	D	240	VAL
1	D	250	ILE
1	D	254	LEU
1	D	258	ARG
1	D	281	LEU
1	D	307	THR
1	D	310	THR
1	D	362	ILE
1	D	378	ASN
1	D	382	LEU
1	D	448	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	38	GLN
1	A	90	GLN
1	A	161	HIS
1	A	175	ASN
1	A	191	ASN
1	A	278	GLN
1	A	279	GLN
1	A	365	GLN
1	B	90	GLN
1	B	175	ASN
1	B	201	GLN
1	B	203	HIS
1	B	278	GLN
1	B	279	GLN
1	B	378	ASN
1	B	392	ASN
1	B	400	ASN
1	B	419	ASN
1	B	439	GLN
1	C	38	GLN
1	C	158	GLN
1	C	175	ASN
1	C	400	ASN
1	C	419	ASN
1	D	90	GLN
1	D	99	ASN
1	D	168	HIS
1	D	175	ASN
1	D	182	GLN
1	D	201	GLN
1	D	278	GLN
1	D	378	ASN
1	D	412	GLN
1	D	414	HIS
1	D	419	ASN
1	D	439	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	433/453 (95%)	0.00	7 (1%) 70 68	30, 57, 92, 109	0
1	B	407/453 (89%)	0.48	29 (7%) 22 19	32, 70, 152, 158	0
1	C	432/453 (95%)	0.35	16 (3%) 45 41	29, 70, 122, 136	0
1	D	409/453 (90%)	0.25	14 (3%) 48 44	31, 61, 128, 143	0
All	All	1681/1812 (92%)	0.27	66 (3%) 43 39	29, 63, 127, 158	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	LEU	5.9
1	C	450	VAL	4.6
1	D	333	LEU	4.1
1	B	340	ALA	4.0
1	D	350	PHE	4.0
1	B	350	PHE	4.0
1	B	403	GLY	3.5
1	B	341	LEU	3.5
1	B	367	ALA	3.4
1	A	331	THR	3.3
1	B	368	ALA	3.3
1	C	10	ALA	3.1
1	C	333	LEU	3.1
1	C	28	GLY	3.0
1	C	332	LEU	3.0
1	A	332	LEU	3.0
1	B	347	PRO	3.0
1	C	31	LEU	2.9
1	C	347	PRO	2.8
1	A	307	THR	2.8
1	D	348	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	339	THR	2.8
1	B	265	ASP	2.7
1	D	331	THR	2.7
1	D	403	GLY	2.6
1	B	363	VAL	2.5
1	A	451	PRO	2.5
1	D	347	PRO	2.5
1	D	341	LEU	2.5
1	B	328	PRO	2.4
1	D	328	PRO	2.4
1	C	377	PRO	2.4
1	B	331	THR	2.4
1	B	416	LEU	2.4
1	D	402	LEU	2.4
1	D	405	ARG	2.4
1	B	241	ALA	2.4
1	B	317	PHE	2.4
1	D	256	LEU	2.3
1	C	246	SER	2.3
1	B	333	LEU	2.3
1	C	309	VAL	2.3
1	B	401	PHE	2.3
1	D	344	LEU	2.3
1	C	253	LEU	2.3
1	A	197	ILE	2.3
1	B	443	ALA	2.3
1	D	107	ALA	2.2
1	B	404	ASP	2.2
1	B	449	LEU	2.2
1	C	328	PRO	2.2
1	B	377	PRO	2.2
1	B	254	LEU	2.2
1	D	349	TRP	2.2
1	C	254	LEU	2.2
1	B	394	ALA	2.1
1	B	364	LEU	2.1
1	B	402	LEU	2.1
1	C	256	LEU	2.1
1	A	8	THR	2.1
1	B	396	LEU	2.1
1	C	302	LEU	2.1
1	C	346	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	202	VAL	2.0
1	B	249	ALA	2.0
1	B	251	ALA	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(Å ²)	Q<0.9
2	MG	C	501	1/1	0.71	0.23	75,75,75,75	0
2	MG	A	501	1/1	0.80	0.18	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.