



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:11 AM UTC

PDB ID : 2WK5 / pdb_00002wk5
Title : Structural features of native human thymidine phosphorylase and in complex with 5-iodouracil
Authors : Mitsiki, E.; Papageorgiou, A.C.; Iyer, S.; Thiagarajan, N.; Prior, S.H.; Sleep, D.; Finnis, C.; Acharya, K.R.
Deposited on : 2009-06-05
Resolution : 2.99 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

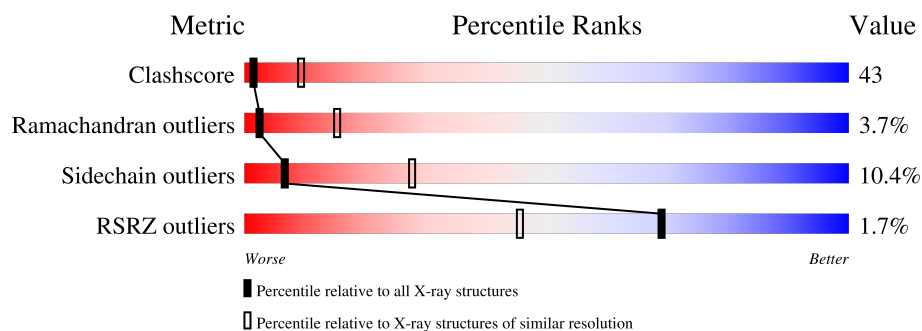
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	482	46% 42% 5% 7%
1	B	482	41% 43% 8% 7%
1	C	482	35% 48% 9% 8%
1	D	482	35% 49% 8% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	1481	-	X	-	-

2 Entry composition [i](#)

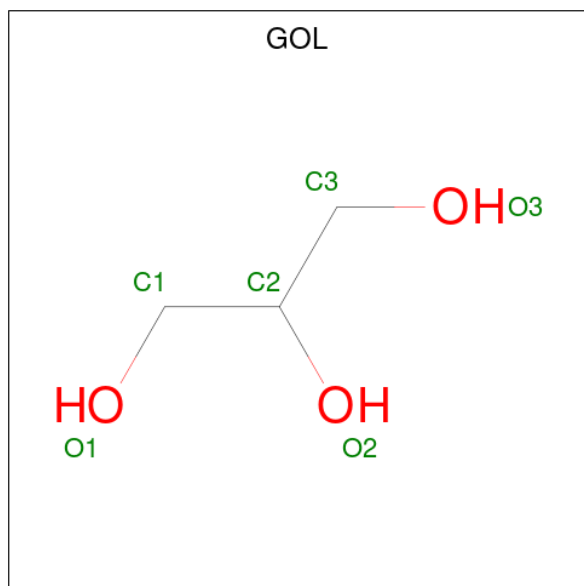
There are 3 unique types of molecules in this entry. The entry contains 13034 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDINE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	1
			3271	2043	600	612	16			
1	B	448	Total	C	N	O	S	0	0	1
			3262	2039	596	611	16			
1	C	445	Total	C	N	O	S	0	0	1
			3243	2023	596	608	16			
1	D	445	Total	C	N	O	S	0	0	1
			3234	2020	592	606	16			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is water.

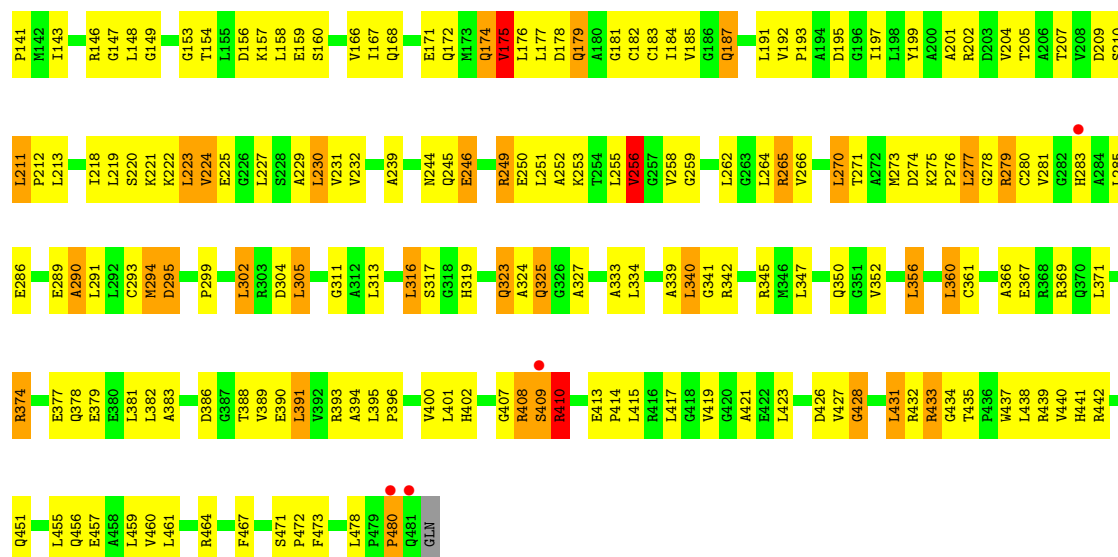
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	B	7	Total 7	O 7	0	0
3	C	2	Total 2	O 2	0	0
3	D	3	Total 3	O 3	0	0

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

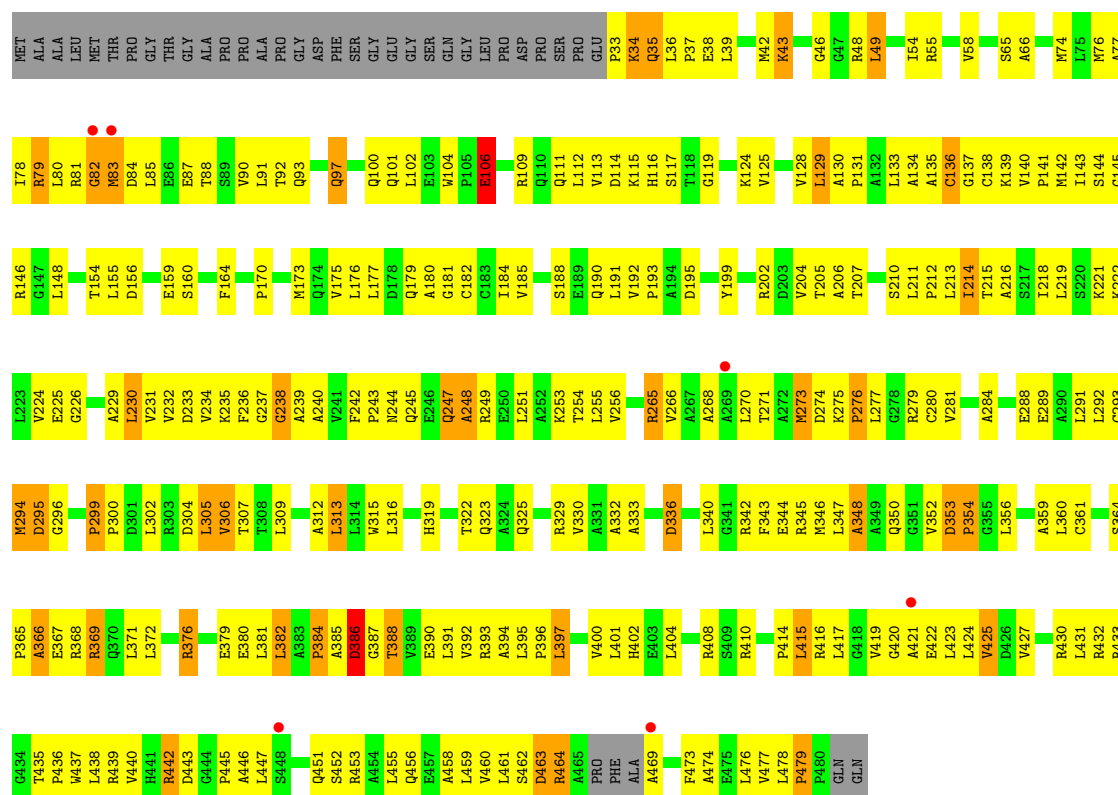
Chain A:

Residue	RMSF (Å)	Chain Segment
P479	0.01	MET
P480	0.01	MET
G1N	0.01	MET
G1N	0.01	MET
V392	0.01	PRO
R393	0.01	PRO
A394	0.01	PRO
L395	0.01	PRO
P396	0.01	PRO
R408	0.01	PRO
S409	0.01	PRO
R410	0.01	PRO
A411	0.01	PRO
G412	0.01	PRO
L415	0.01	PRO
G418	0.01	PRO
L423	0.01	PRO
L424	0.01	PRO
V425	0.01	PRO
D426	0.01	PRO
V427	0.01	PRO
G428	0.01	PRO
Q429	0.01	PRO
R430	0.01	PRO
L431	0.01	PRO
R432	0.01	PRO
R433	0.01	PRO
G434	0.01	PRO
T435	0.01	PRO
P436	0.01	PRO
V437	0.01	PRO
L438	0.01	PRO
R439	0.01	PRO
H441	0.01	PRO
R442	0.01	PRO
P445	0.01	PRO
A446	0.01	PRO
R453	0.01	PRO
Q456	0.01	SER
E457	0.01	SER
A458	0.01	SER
L459	0.01	SER
V460	0.01	SER
L461	0.01	SER
S462	0.01	SER
D463	0.01	SER
R464	0.01	SER
F467	0.01	SER
P472	0.01	SER
F473	0.01	SER
L476	0.01	SER
V477	0.01	SER
L478	0.01	SER
L158	0.02	MET
G237	0.02	MET
G238	0.02	MET
E159	0.02	MET
S160	0.02	MET
D84	0.02	MET
F164	0.02	PRO
N165	0.02	PRO
Q168	0.02	PRO
S169	0.02	PRO
L191	0.02	PRO
P170	0.02	PRO
M173	0.02	PRO
L176	0.02	PRO
L177	0.02	PRO
C183	0.02	PRO
I184	0.02	PRO
V185	0.02	PRO
Q190	0.02	PRO
V192	0.02	PRO
P193	0.02	PRO
Y199	0.02	PRO
R202	0.02	PRO
D203	0.02	PRO
V204	0.02	PRO
A206	0.02	PRO
T207	0.02	PRO
V208	0.02	PRO
D209	0.02	PRO
S210	0.02	PRO
L211	0.02	PRO
P212	0.02	PRO
L213	0.02	PRO
I214	0.02	PRO
T215	0.02	PRO
A216	0.02	PRO
S217	0.02	PRO
L218	0.02	PRO
L219	0.02	PRO
L223	0.02	PRO
V224	0.02	PRO
E225	0.02	PRO
G226	0.02	PRO
L227	0.02	PRO
S228	0.02	PRO
A229	0.02	PRO
L230	0.02	PRO
V231	0.02	PRO
V232	0.02	PRO
D233	0.02	PRO
V234	0.02	PRO
K235	0.02	PRO
F236	0.02	PRO
G237	0.02	SER
G238	0.02	SER
V241	0.02	SER
F242	0.02	SER
P243	0.02	SER
N244	0.02	SER
Q245	0.02	SER
E246	0.02	SER
Q247	0.02	SER
A248	0.02	SER
R249	0.02	SER
E250	0.02	SER
L251	0.02	SER
A252	0.02	SER
K253	0.02	SER
T254	0.02	SER
L255	0.02	SER
V256	0.02	SER
G257	0.02	SER
L262	0.02	SER
R265	0.02	SER
V266	0.02	SER
A267	0.02	SER
A268	0.02	SER
A269	0.02	SER
L270	0.02	SER
F273	0.02	SER
L274	0.02	SER
L277	0.02	SER
G278	0.02	SER
R279	0.02	SER

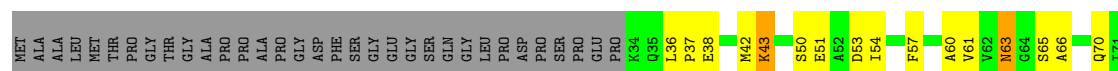
[illegible]



• Molecule 1: THYMIDINE PHOSPHORYLASE



• Molecule 1: THYMIDINE PHOSPHORYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.53Å 77.19Å 100.88Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	42.61 – 2.99 42.61 – 2.99	Depositor EDS
% Data completeness (in resolution range)	85.2 (42.61-2.99) 81.3 (42.61-2.99)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.207 , 0.284 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13034	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6072e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL

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	0.54	1/3318 (0.0%)	1.04	12/4502 (0.3%)
1	B	0.54	1/3309 (0.0%)	1.04	17/4490 (0.4%)
1	C	0.47	1/3287 (0.0%)	1.03	15/4456 (0.3%)
1	D	0.50	1/3278 (0.0%)	1.03	12/4446 (0.3%)
All	All	0.52	4/13192 (0.0%)	1.03	56/17894 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	480	PRO	C-N	-5.67	1.25	1.33
1	D	479	PRO	C-N	-5.47	1.25	1.34
1	C	479	PRO	C-N	-5.46	1.25	1.34
1	A	479	PRO	C-N	-5.38	1.25	1.34

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	140	VAL	N-CA-C	8.50	116.56	108.15
1	B	140	VAL	N-CA-C	8.14	116.20	108.15
1	D	189	GLU	N-CA-C	-7.67	103.18	112.54
1	C	366	ALA	N-CA-C	-7.35	103.35	111.36
1	B	251	LEU	N-CA-C	-7.08	103.64	111.36
1	A	335	ASP	N-CA-C	7.03	119.97	111.82
1	A	256	VAL	N-CA-C	-6.81	103.84	110.72
1	C	129	LEU	N-CA-C	6.77	118.32	111.07
1	B	51	GLU	N-CA-C	-6.51	105.06	112.87
1	B	156	ASP	N-CA-C	-6.24	104.56	111.36
1	C	248	ALA	N-CA-C	-6.24	105.77	113.19
1	B	79	ARG	N-CA-C	6.23	117.87	111.14
1	A	248	ALA	N-CA-C	-6.19	105.38	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	302	LEU	N-CA-C	-6.14	104.51	111.14
1	A	160	SER	N-CA-C	-6.08	104.21	111.69
1	C	106	GLU	N-CA-C	-6.06	104.60	112.23
1	D	151	THR	N-CA-C	-6.06	101.24	110.14
1	B	62	VAL	N-CA-C	5.92	116.10	110.53
1	B	179	GLN	N-CA-C	5.89	117.50	111.14
1	D	339	ALA	N-CA-C	-5.81	104.86	111.07
1	A	140	VAL	N-CA-C	5.80	113.90	108.15
1	A	266	VAL	N-CA-C	5.79	116.45	108.12
1	B	410	ARG	N-CA-C	5.73	118.39	111.40
1	B	294	MET	N-CA-C	-5.72	106.07	113.16
1	B	325	GLN	N-CA-C	-5.70	104.27	111.11
1	B	428	GLY	N-CA-C	-5.69	107.92	114.69
1	B	290	ALA	N-CA-C	-5.64	105.22	111.36
1	C	294	MET	N-CA-C	-5.60	105.33	111.82
1	C	353	ASP	CA-C-N	5.59	126.83	119.84
1	C	353	ASP	C-N-CA	5.59	126.83	119.84
1	D	109	ARG	N-CA-C	5.53	118.82	111.75
1	D	287	VAL	CB-CA-C	-5.51	104.92	111.81
1	B	175	VAL	N-CA-C	-5.49	105.17	110.72
1	A	142	MET	N-CA-C	5.48	117.23	108.41
1	B	323	GLN	N-CA-C	-5.44	105.43	111.36
1	C	65	SER	N-CA-C	-5.44	106.15	112.89
1	C	299	PRO	CA-C-N	5.40	125.05	119.05
1	C	299	PRO	C-N-CA	5.40	125.05	119.05
1	D	284	ALA	N-CA-C	-5.29	105.51	111.28
1	C	293	CYS	N-CA-C	-5.23	105.66	111.36
1	A	206	ALA	N-CA-C	-5.21	104.70	111.74
1	B	274	ASP	N-CA-C	-5.20	106.08	112.90
1	D	72	GLY	N-CA-C	-5.19	106.20	112.49
1	D	399	LEU	N-CA-C	5.17	117.33	111.02
1	C	247	GLN	N-CA-C	-5.13	106.35	113.18
1	A	98	SER	N-CA-C	-5.13	106.28	112.54
1	C	315	TRP	N-CA-C	-5.13	105.38	110.97
1	A	458	ALA	N-CA-C	-5.10	107.00	113.18
1	C	336	ASP	N-CA-C	5.09	119.24	113.19
1	C	348	ALA	N-CA-C	-5.08	105.93	111.82
1	D	178	ASP	N-CA-C	-5.07	106.33	112.88
1	B	256	VAL	N-CA-C	-5.05	105.49	111.00
1	D	443	ASP	N-CA-C	-5.05	107.67	113.88
1	A	242	PHE	CA-C-N	5.03	126.13	119.84
1	A	242	PHE	C-N-CA	5.03	126.13	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	323	GLN	N-CA-C	-5.03	105.80	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3271	0	3364	221	0
1	B	3262	0	3352	277	0
1	C	3243	0	3341	344	0
1	D	3234	0	3311	308	0
2	B	6	0	4	0	0
3	A	6	0	0	0	0
3	B	7	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
All	All	13034	0	13372	1145	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 43.

All (1145) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:GLY:O	1:D:368:ARG:NH1	1.57	1.37
1:B:408:ARG:HG3	1:B:413:GLU:CG	1.65	1.26
1:B:408:ARG:HG3	1:B:413:GLU:HG2	1.22	1.20
1:B:102:LEU:HD22	1:B:104:TRP:CZ2	1.78	1.18
1:C:386:ASP:HB2	1:C:432:ARG:HA	1.30	1.14
1:D:364:SER:O	1:D:368:ARG:NH1	1.80	1.13
1:B:283:HIS:NE2	1:B:415:LEU:HD23	1.64	1.12
1:C:92:THR:HG22	1:C:216:ALA:HA	1.29	1.10
1:C:464:ARG:HG3	1:C:464:ARG:HH11	1.15	1.07
1:D:164:PHE:CZ	1:D:350:GLN:OE1	2.07	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:HIS:CE1	1:B:415:LEU:HD23	1.91	1.05
1:A:100:GLN:HE21	1:A:190:GLN:HB3	1.17	1.02
1:A:426:ASP:H	1:A:429:GLN:HE21	1.07	1.02
1:C:230:LEU:HD12	1:C:266:VAL:HG12	1.38	1.00
1:D:245:GLN:H	1:D:245:GLN:NE2	1.60	1.00
1:C:369:ARG:HH11	1:C:369:ARG:HB2	1.24	0.99
1:C:386:ASP:HB2	1:C:432:ARG:CA	1.92	0.99
1:D:163:GLY:O	1:D:351:GLY:O	1.81	0.98
1:C:464:ARG:HH11	1:C:464:ARG:CG	1.76	0.98
1:A:285:LEU:HD12	1:A:285:LEU:H	1.28	0.96
1:B:187:GLN:H	1:B:187:GLN:HE21	0.98	0.95
1:B:408:ARG:HG3	1:B:413:GLU:HG3	1.46	0.95
1:C:211:LEU:HD11	1:C:254:THR:HG21	1.48	0.95
1:D:130:ALA:HB3	1:D:131:PRO:HD3	1.49	0.95
1:D:456:GLN:HE21	1:D:456:GLN:HA	1.33	0.93
1:D:83:MET:HE3	1:D:87:GLU:HB3	1.49	0.93
1:D:322:THR:HG23	1:D:325:GLN:H	1.33	0.93
1:B:187:GLN:H	1:B:187:GLN:NE2	1.67	0.92
1:A:322:THR:HG22	1:A:325:GLN:HG3	1.48	0.92
1:A:223:LEU:HD11	1:A:262:LEU:HD13	1.51	0.91
1:D:347:LEU:O	1:D:352:VAL:HG23	1.71	0.91
1:D:124:LYS:HG3	1:D:302:LEU:HD21	1.50	0.91
1:D:120:GLY:HA3	1:D:273:MET:HE3	1.50	0.91
1:D:141:PRO:HA	1:D:183:CYS:SG	2.11	0.91
1:B:381:LEU:HD12	1:B:438:LEU:HD23	1.51	0.91
1:C:229:ALA:HB1	1:C:316:LEU:HD12	1.51	0.91
1:C:170:PRO:HA	1:C:173:MET:HE3	1.53	0.90
1:A:130:ALA:HB3	1:A:131:PRO:HD3	1.53	0.90
1:C:386:ASP:CB	1:C:432:ARG:HA	2.02	0.90
1:D:365:PRO:O	1:D:368:ARG:N	2.04	0.90
1:B:279:ARG:HG2	1:B:423:LEU:O	1.73	0.89
1:D:101:GLN:HE21	1:D:224:VAL:HG22	1.37	0.89
1:D:356:LEU:HD22	1:D:371:LEU:HD23	1.54	0.89
1:C:101:GLN:HE21	1:C:224:VAL:HG22	1.36	0.89
1:C:210:SER:HB3	1:C:213:LEU:HB2	1.55	0.89
1:A:79:ARG:O	1:A:79:ARG:HD3	1.72	0.88
1:C:33:PRO:O	1:C:34:LYS:HG3	1.73	0.88
1:A:229:ALA:HB1	1:A:316:LEU:HD12	1.53	0.88
1:C:55:ARG:HH12	1:C:97:GLN:HE22	1.16	0.88
1:B:402:HIS:NE2	1:B:409:SER:HB2	1.89	0.88
1:B:102:LEU:HD22	1:B:104:TRP:CE2	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:ARG:NH1	1:C:97:GLN:HE22	1.73	0.87
1:B:381:LEU:HB3	1:B:456:GLN:HE22	1.38	0.86
1:C:48:ARG:HD2	1:C:84:ASP:OD2	1.75	0.86
1:D:93:GLN:O	1:D:97:GLN:HG2	1.75	0.86
1:D:289:GLU:OE1	1:D:299:PRO:HG2	1.76	0.86
1:A:63:ASN:HD22	1:A:64:GLY:N	1.72	0.86
1:C:453:ARG:HH11	1:C:453:ARG:HB3	1.41	0.85
1:D:162:PRO:O	1:D:352:VAL:HG13	1.76	0.85
1:D:163:GLY:C	1:D:351:GLY:O	2.20	0.85
1:B:109:ARG:HA	1:B:112:LEU:HD12	1.59	0.85
1:B:408:ARG:CG	1:B:413:GLU:HG2	2.06	0.84
1:C:453:ARG:HB3	1:C:453:ARG:NH1	1.92	0.84
1:A:100:GLN:NE2	1:A:190:GLN:HB3	1.91	0.84
1:C:271:THR:HG21	1:C:305:LEU:HD21	1.58	0.84
1:B:366:ALA:CB	1:D:99:GLY:HA2	2.07	0.84
1:A:118:THR:OG1	1:A:119:GLY:N	2.09	0.84
1:B:63:ASN:C	1:B:63:ASN:HD22	1.85	0.84
1:D:76:MET:HE2	1:D:80:LEU:HG	1.60	0.84
1:B:374:ARG:HH11	1:B:374:ARG:CG	1.89	0.83
1:B:249:ARG:HH11	1:B:249:ARG:HB3	1.41	0.83
1:B:431:LEU:HD21	1:B:435:THR:HB	1.59	0.83
1:D:291:LEU:HD13	1:D:368:ARG:HE	1.43	0.83
1:C:173:MET:HE2	1:C:191:LEU:HD11	1.59	0.83
1:C:173:MET:HA	1:C:176:LEU:HD12	1.60	0.83
1:D:463:ASP:O	1:D:464:ARG:C	2.16	0.82
1:B:285:LEU:HD21	1:B:369:ARG:NH2	1.94	0.82
1:C:393:ARG:CB	1:C:458:ALA:HA	2.09	0.82
1:A:118:THR:O	1:A:119:GLY:O	1.98	0.82
1:C:386:ASP:HB2	1:C:433:ARG:N	1.94	0.82
1:B:102:LEU:CD2	1:B:104:TRP:CZ2	2.63	0.81
1:C:393:ARG:HG3	1:C:396:PRO:CD	2.10	0.81
1:D:294:MET:HE1	1:D:343:PHE:HB2	1.61	0.81
1:D:245:GLN:H	1:D:245:GLN:CD	1.88	0.81
1:D:422:GLU:HB2	1:D:439:ARG:HB3	1.63	0.81
1:B:374:ARG:HH11	1:B:374:ARG:HG3	1.46	0.80
1:D:463:ASP:O	1:D:464:ARG:O	1.99	0.80
1:A:75:LEU:HB3	1:A:207:THR:HG21	1.63	0.80
1:A:88:THR:O	1:A:92:THR:HG22	1.80	0.80
1:D:79:ARG:HG3	1:D:207:THR:HA	1.64	0.80
1:C:416:ARG:NH1	1:C:443:ASP:HB3	1.96	0.80
1:D:84:ASP:OD2	1:D:87:GLU:HG3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:THR:HG22	1:C:216:ALA:CA	2.09	0.80
1:B:175:VAL:HG22	1:B:179:GLN:HE21	1.46	0.80
1:C:395:LEU:HB3	1:C:396:PRO:HD3	1.63	0.79
1:B:374:ARG:HG3	1:B:374:ARG:NH1	1.97	0.79
1:D:395:LEU:HB3	1:D:396:PRO:HD3	1.65	0.79
1:C:397:LEU:O	1:C:401:LEU:HD23	1.83	0.79
1:C:478:LEU:HD12	1:C:479:PRO:HD2	1.64	0.79
1:B:395:LEU:HB3	1:B:396:PRO:HD3	1.64	0.79
1:A:428:GLY:HA2	1:A:467:PHE:CE2	2.18	0.78
1:B:49:LEU:HB2	1:B:54:ILE:HD11	1.64	0.78
1:B:166:VAL:HG23	1:B:167:ILE:HD12	1.66	0.78
1:B:83:MET:HE2	1:B:87:GLU:HB3	1.65	0.78
1:C:294:MET:HB3	1:C:340:LEU:HB2	1.64	0.78
1:A:104:TRP:H	1:A:109:ARG:HH12	1.30	0.78
1:C:249:ARG:HH12	1:C:253:LYS:HE2	1.47	0.78
1:B:131:PRO:HB2	1:B:294:MET:HE1	1.66	0.78
1:B:283:HIS:CE1	1:B:415:LEU:CD2	2.67	0.78
1:B:366:ALA:HB1	1:D:99:GLY:HA2	1.66	0.77
1:B:112:LEU:HD23	1:B:139:LYS:HB3	1.65	0.77
1:B:381:LEU:HB3	1:B:456:GLN:NE2	1.98	0.77
1:A:63:ASN:HD22	1:A:63:ASN:C	1.91	0.77
1:B:139:LYS:HG3	1:B:177:LEU:HD13	1.66	0.77
1:B:239:ALA:HB3	1:B:273:MET:HG3	1.67	0.77
1:C:274:ASP:O	1:C:394:ALA:HB3	1.84	0.77
1:C:427:VAL:CG1	1:C:469:ALA:HB2	2.16	0.76
1:B:79:ARG:HG3	1:B:207:THR:HG22	1.68	0.76
1:A:453:ARG:HB3	1:B:179:GLN:OE1	1.84	0.76
1:B:177:LEU:O	1:B:181:GLY:HA2	1.86	0.76
1:D:291:LEU:HB3	1:D:368:ARG:HH21	1.52	0.76
1:C:416:ARG:HH11	1:C:443:ASP:HB3	1.48	0.75
1:D:390:GLU:CG	1:D:462:SER:OG	2.34	0.75
1:B:187:GLN:HE21	1:B:187:GLN:N	1.79	0.75
1:B:381:LEU:HD13	1:B:456:GLN:HE21	1.52	0.75
1:C:386:ASP:HB2	1:C:433:ARG:H	1.48	0.75
1:B:431:LEU:HD23	1:B:432:ARG:H	1.50	0.75
1:B:102:LEU:CD1	1:B:225:GLU:HA	2.17	0.75
1:B:249:ARG:HH11	1:B:249:ARG:CB	1.99	0.74
1:B:283:HIS:NE2	1:B:415:LEU:CD2	2.48	0.74
1:B:63:ASN:ND2	1:B:65:SER:H	1.86	0.74
1:D:405:GLY:HA3	1:D:416:ARG:HG3	1.70	0.74
1:A:143:ILE:HG13	1:A:225:GLU:OE1	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:GLY:HA3	1:B:266:VAL:HG21	1.69	0.74
1:A:294:MET:O	1:A:295:ASP:O	2.06	0.74
1:C:442:ARG:NH2	1:C:446:ALA:HA	2.03	0.74
1:D:463:ASP:C	1:D:464:ARG:O	2.28	0.74
1:A:63:ASN:ND2	1:A:65:SER:H	1.85	0.74
1:B:146:ARG:NH1	1:B:159:GLU:OE2	2.20	0.74
1:D:230:LEU:HD12	1:D:266:VAL:HG13	1.68	0.73
1:A:92:THR:HB	1:A:216:ALA:HA	1.69	0.73
1:C:386:ASP:CB	1:C:433:ARG:H	2.00	0.73
1:C:393:ARG:HB2	1:C:458:ALA:HA	1.68	0.73
1:B:431:LEU:CD2	1:B:435:THR:HB	2.19	0.73
1:B:184:ILE:H	1:B:350:GLN:HE22	1.37	0.72
1:D:161:ILE:HD11	1:D:287:VAL:HG11	1.71	0.72
1:B:49:LEU:HB2	1:B:54:ILE:CD1	2.18	0.72
1:C:401:LEU:HD13	1:C:404:LEU:HD12	1.70	0.72
1:A:79:ARG:HB2	1:A:207:THR:HG23	1.70	0.72
1:A:176:LEU:HD21	1:A:350:GLN:HG3	1.70	0.72
1:A:392:VAL:HG21	1:A:423:LEU:HD11	1.71	0.72
1:C:88:THR:O	1:C:92:THR:HG23	1.90	0.72
1:C:381:LEU:O	1:C:437:TRP:NE1	2.23	0.71
1:D:356:LEU:HD13	1:D:356:LEU:O	1.90	0.71
1:B:377:GLU:HB3	1:B:442:ARG:HH22	1.55	0.71
1:D:456:GLN:HA	1:D:456:GLN:NE2	2.05	0.71
1:D:167:ILE:HD12	1:D:167:ILE:H	1.53	0.71
1:D:239:ALA:HB3	1:D:273:MET:HG3	1.72	0.71
1:A:408:ARG:NE	1:A:415:LEU:HD13	2.05	0.71
1:D:390:GLU:OE2	1:D:464:ARG:CD	2.39	0.71
1:C:173:MET:CE	1:C:191:LEU:HD11	2.20	0.71
1:A:234:VAL:HB	1:A:270:LEU:HD23	1.73	0.71
1:A:410:ARG:O	1:A:410:ARG:HG2	1.91	0.71
1:C:55:ARG:HH12	1:C:97:GLN:NE2	1.88	0.71
1:C:401:LEU:HA	1:C:404:LEU:HD12	1.71	0.71
1:B:249:ARG:HB3	1:B:249:ARG:NH1	2.04	0.70
1:C:390:GLU:HG3	1:C:462:SER:HB3	1.71	0.70
1:C:268:ALA:HB3	1:C:477:VAL:HB	1.70	0.70
1:C:393:ARG:HG2	1:C:393:ARG:HH11	1.55	0.70
1:A:211:LEU:HD21	1:A:254:THR:HG21	1.73	0.70
1:B:135:ALA:HA	1:B:342:ARG:NE	2.06	0.70
1:D:96:ALA:O	1:D:101:GLN:NE2	2.20	0.70
1:B:175:VAL:HG22	1:B:179:GLN:NE2	2.05	0.70
1:C:422:GLU:OE1	1:C:439:ARG:HD2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:PRO:O	1:D:366:ALA:C	2.33	0.70
1:B:130:ALA:HB3	1:B:131:PRO:HD3	1.72	0.70
1:D:60:ALA:HA	1:D:63:ASN:HD21	1.54	0.70
1:D:93:GLN:HB3	1:D:97:GLN:HE21	1.55	0.70
1:D:244:ASN:HB3	1:D:247:GLN:HB3	1.72	0.70
1:B:154:THR:HA	1:B:157:LYS:HD2	1.74	0.70
1:B:408:ARG:CG	1:B:413:GLU:CG	2.58	0.70
1:C:289:GLU:OE2	1:C:299:PRO:HG2	1.91	0.69
1:B:408:ARG:O	1:B:408:ARG:HG2	1.92	0.69
1:D:101:GLN:NE2	1:D:224:VAL:HG22	2.07	0.69
1:C:381:LEU:O	1:C:437:TRP:CD1	2.45	0.69
1:C:392:VAL:HA	1:C:458:ALA:O	1.92	0.69
1:C:459:LEU:HD22	1:C:461:LEU:HG	1.73	0.69
1:C:111:GLN:HE21	1:C:319:HIS:CE1	2.10	0.69
1:C:369:ARG:HB2	1:C:369:ARG:NH1	2.04	0.69
1:B:205:THR:HG22	1:B:205:THR:O	1.92	0.69
1:A:445:PRO:O	1:A:446:ALA:HB2	1.93	0.69
1:B:408:ARG:HB3	1:B:415:LEU:HD11	1.73	0.69
1:C:464:ARG:CG	1:C:464:ARG:NH1	2.45	0.69
1:D:379:GLU:OE1	1:D:447:LEU:HG	1.93	0.69
1:A:205:THR:HG22	1:A:207:THR:OG1	1.93	0.69
1:D:202:ARG:HD2	1:D:213:LEU:HD22	1.73	0.69
1:D:390:GLU:HG3	1:D:462:SER:OG	1.93	0.69
1:D:416:ARG:NH1	1:D:443:ASP:OD1	2.24	0.69
1:A:123:ASP:OD2	1:A:277:LEU:HD12	1.94	0.68
1:A:426:ASP:O	1:A:429:GLN:HG2	1.92	0.68
1:C:135:ALA:HA	1:C:342:ARG:NH1	2.08	0.68
1:A:322:THR:CG2	1:A:325:GLN:HG3	2.23	0.68
1:A:235:LYS:HE3	1:A:273:MET:HG2	1.75	0.68
1:C:102:LEU:HD21	1:C:173:MET:HE3	1.75	0.68
1:C:130:ALA:HB3	1:C:131:PRO:HD3	1.76	0.68
1:C:249:ARG:NH1	1:C:253:LYS:HE2	2.09	0.68
1:C:101:GLN:NE2	1:C:224:VAL:HG22	2.09	0.68
1:B:172:GLN:O	1:B:176:LEU:HD23	1.93	0.68
1:A:437:TRP:CE3	1:A:459:LEU:HD23	2.28	0.68
1:D:347:LEU:O	1:D:352:VAL:CG2	2.42	0.68
1:B:378:GLN:NE2	1:B:439:ARG:HD3	2.09	0.68
1:D:223:LEU:HD11	1:D:262:LEU:HB3	1.75	0.67
1:B:74:MET:HE3	1:B:77:ALA:HB3	1.75	0.67
1:C:386:ASP:HB2	1:C:432:ARG:C	2.19	0.67
1:A:370:GLN:HG2	1:A:374:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:THR:O	1:D:206:ALA:HB3	1.93	0.67
1:C:211:LEU:CD1	1:C:254:THR:HG21	2.23	0.67
1:C:249:ARG:HH12	1:C:253:LYS:CE	2.07	0.67
1:C:386:ASP:CB	1:C:433:ARG:N	2.58	0.67
1:D:36:LEU:HD11	1:D:57:PHE:HD1	1.59	0.67
1:A:124:LYS:H	1:A:124:LYS:HD2	1.58	0.67
1:B:34:LYS:HE3	1:B:42:MET:HE2	1.77	0.67
1:A:294:MET:O	1:A:295:ASP:C	2.37	0.66
1:A:391:LEU:HA	1:A:427:VAL:HG22	1.77	0.66
1:D:106:GLU:HA	1:D:109:ARG:HH11	1.60	0.66
1:D:326:GLY:O	1:D:330:VAL:HG23	1.95	0.66
1:A:34:LYS:HE2	1:A:42:MET:HE1	1.76	0.66
1:A:442:ARG:CZ	1:A:446:ALA:HA	2.25	0.66
1:C:230:LEU:HD12	1:C:266:VAL:CG1	2.21	0.66
1:C:393:ARG:HG3	1:C:396:PRO:CG	2.25	0.66
1:D:161:ILE:HG21	1:D:347:LEU:HD22	1.78	0.66
1:A:285:LEU:H	1:A:285:LEU:CD1	2.05	0.66
1:C:133:LEU:HD11	1:C:313:LEU:HD12	1.78	0.66
1:C:343:PHE:CE2	1:C:347:LEU:HD11	2.31	0.66
1:D:192:VAL:HG13	1:D:224:VAL:HG21	1.77	0.66
1:C:54:ILE:O	1:C:58:VAL:HG23	1.95	0.66
1:D:210:SER:HB3	1:D:213:LEU:HB2	1.78	0.66
1:D:106:GLU:HA	1:D:109:ARG:HD3	1.78	0.66
1:C:478:LEU:CD1	1:C:479:PRO:HD2	2.26	0.66
1:D:368:ARG:C	1:D:370:GLN:H	2.04	0.66
1:C:393:ARG:HB3	1:C:458:ALA:HA	1.78	0.65
1:D:270:LEU:HB2	1:D:474:ALA:HB3	1.78	0.65
1:C:427:VAL:HG11	1:C:469:ALA:HB2	1.76	0.65
1:C:464:ARG:HG3	1:C:464:ARG:NH1	1.97	0.65
1:D:330:VAL:O	1:D:334:LEU:HG	1.96	0.65
1:C:300:PRO:O	1:C:304:ASP:HB2	1.96	0.65
1:D:365:PRO:HA	1:D:368:ARG:HD3	1.79	0.65
1:B:55:ARG:HH12	1:B:97:GLN:HE22	1.45	0.65
1:C:279:ARG:HG2	1:C:279:ARG:HH21	1.61	0.65
1:C:83:MET:CB	1:C:87:GLU:OE2	2.45	0.65
1:D:276:PRO:HG2	1:D:397:LEU:HD23	1.77	0.65
1:D:376:ARG:HB3	1:D:443:ASP:HA	1.79	0.65
1:D:385:ALA:HA	1:D:433:ARG:HB2	1.78	0.65
1:C:422:GLU:HB3	1:C:439:ARG:HB3	1.79	0.65
1:D:390:GLU:OE2	1:D:464:ARG:HD3	1.96	0.65
1:B:89:SER:O	1:B:92:THR:HG22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:GLU:HG2	1:D:462:SER:OG	1.96	0.65
1:B:285:LEU:CD2	1:B:369:ARG:NH2	2.59	0.65
1:D:367:GLU:OE1	1:D:371:LEU:HD11	1.97	0.65
1:A:165:ASN:HB3	1:A:168:GLN:HE22	1.61	0.65
1:C:124:LYS:H	1:C:124:LYS:HD2	1.62	0.65
1:D:164:PHE:HZ	1:D:350:GLN:OE1	1.77	0.65
1:C:55:ARG:NH1	1:C:97:GLN:NE2	2.42	0.64
1:B:408:ARG:HB3	1:B:415:LEU:CD1	2.26	0.64
1:A:442:ARG:NE	1:A:446:ALA:HA	2.12	0.64
1:D:230:LEU:HD13	1:D:231:VAL:N	2.12	0.64
1:C:388:THR:HA	1:C:430:ARG:CB	2.27	0.64
1:C:393:ARG:HG3	1:C:396:PRO:HG2	1.79	0.64
1:D:88:THR:O	1:D:92:THR:HG23	1.98	0.64
1:A:395:LEU:HB3	1:A:396:PRO:HD3	1.79	0.64
1:A:428:GLY:HA2	1:A:467:PHE:CZ	2.33	0.64
1:C:256:VAL:HG22	1:C:479:PRO:HB3	1.78	0.64
1:A:115:LYS:HA	1:A:231:VAL:O	1.97	0.64
1:C:113:VAL:HB	1:C:313:LEU:HD11	1.78	0.64
1:D:60:ALA:HA	1:D:65:SER:HB3	1.80	0.64
1:C:380:GLU:OE2	1:C:436:PRO:HB3	1.98	0.64
1:A:459:LEU:CD1	1:A:461:LEU:HG	2.28	0.64
1:D:83:MET:HE3	1:D:87:GLU:CB	2.24	0.63
1:A:83:MET:HE1	1:A:91:LEU:HD12	1.79	0.63
1:A:269:ALA:HB2	1:A:476:LEU:HD12	1.81	0.63
1:D:50:SER:H	1:D:53:ASP:HB2	1.62	0.63
1:C:202:ARG:HH12	1:C:214:ILE:HG12	1.64	0.63
1:C:322:THR:OG1	1:C:325:GLN:HB2	1.97	0.63
1:D:164:PHE:N	1:D:352:VAL:HG22	2.12	0.63
1:B:102:LEU:HD13	1:B:225:GLU:HA	1.79	0.63
1:B:341:GLY:O	1:B:345:ARG:HD3	1.97	0.63
1:C:36:LEU:HD23	1:C:39:LEU:HD12	1.81	0.63
1:C:464:ARG:NH1	1:C:464:ARG:CB	2.61	0.63
1:D:244:ASN:HD22	1:D:245:GLN:N	1.96	0.63
1:A:340:LEU:HD22	1:A:361:CYS:HB3	1.81	0.63
1:D:467:PHE:N	1:D:467:PHE:CD1	2.67	0.63
1:C:388:THR:HG23	1:C:430:ARG:HB3	1.79	0.63
1:B:275:LYS:HE2	1:B:276:PRO:O	1.99	0.63
1:D:352:VAL:O	1:D:353:ASP:C	2.41	0.63
1:A:392:VAL:HG21	1:A:423:LEU:CD1	2.29	0.62
1:B:183:CYS:HB2	1:B:350:GLN:NE2	2.13	0.62
1:C:54:ILE:HG21	1:C:90:VAL:HG12	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:MET:HE3	1:D:76:MET:HA	1.81	0.62
1:B:442:ARG:HG3	1:B:442:ARG:HH21	1.63	0.62
1:C:145:GLY:C	1:C:155:LEU:HD12	2.24	0.62
1:D:390:GLU:OE2	1:D:464:ARG:HD2	1.99	0.62
1:A:329:ARG:O	1:A:332:ALA:HB3	1.99	0.62
1:B:113:VAL:HG11	1:B:317:SER:HB2	1.81	0.62
1:C:115:LYS:HA	1:C:231:VAL:O	1.99	0.62
1:B:98:SER:HB2	1:B:193:PRO:HD2	1.80	0.62
1:B:222:LYS:HD3	1:B:225:GLU:OE2	1.98	0.62
1:C:381:LEU:HD11	1:C:455:LEU:HD23	1.81	0.62
1:C:431:LEU:H	1:C:431:LEU:HD23	1.64	0.62
1:D:57:PHE:O	1:D:61:VAL:HG23	2.00	0.62
1:D:193:PRO:O	1:D:197:ILE:HG12	1.99	0.62
1:B:43:LYS:CB	1:B:74:MET:HE1	2.30	0.62
1:D:93:GLN:HE21	1:D:262:LEU:HD21	1.64	0.62
1:B:102:LEU:HD12	1:B:225:GLU:HA	1.82	0.62
1:C:242:PHE:C	1:C:244:ASN:H	2.07	0.62
1:A:128:VAL:O	1:A:131:PRO:HD2	2.00	0.62
1:A:408:ARG:HE	1:A:415:LEU:HD13	1.64	0.62
1:D:93:GLN:HB3	1:D:97:GLN:NE2	2.14	0.62
1:B:55:ARG:HH12	1:B:97:GLN:NE2	1.97	0.61
1:D:128:VAL:HG13	1:D:294:MET:HG2	1.82	0.61
1:C:156:ASP:O	1:C:159:GLU:HB2	2.01	0.61
1:B:381:LEU:HD13	1:B:456:GLN:NE2	2.14	0.61
1:A:129:LEU:O	1:A:133:LEU:HG	2.00	0.61
1:C:83:MET:HB3	1:C:87:GLU:OE2	2.00	0.61
1:C:379:GLU:OE1	1:C:447:LEU:HG	2.01	0.61
1:D:371:LEU:H	1:D:371:LEU:HD12	1.65	0.61
1:B:168:GLN:HG3	1:B:185:VAL:HG11	1.82	0.61
1:B:239:ALA:HB2	1:B:394:ALA:HB3	1.82	0.61
1:D:416:ARG:HB2	1:D:419:VAL:HG23	1.82	0.61
1:C:288:GLU:HG2	1:C:372:LEU:HD12	1.82	0.61
1:D:291:LEU:HD13	1:D:368:ARG:NE	2.16	0.61
1:C:231:VAL:HG23	1:C:313:LEU:HD23	1.82	0.61
1:C:102:LEU:HD21	1:C:173:MET:CE	2.30	0.60
1:B:128:VAL:HG13	1:B:294:MET:HE3	1.83	0.60
1:C:265:ARG:HD2	1:C:316:LEU:HD11	1.83	0.60
1:D:265:ARG:NH2	1:D:316:LEU:O	2.35	0.60
1:D:280:CYS:HB2	1:D:289:GLU:OE2	2.01	0.60
1:A:104:TRP:H	1:A:109:ARG:NH1	1.99	0.60
1:A:245:GLN:O	1:A:248:ALA:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:ARG:HH11	1:C:369:ARG:CB	2.09	0.60
1:D:288:GLU:HG2	1:D:372:LEU:HD12	1.84	0.60
1:A:277:LEU:HD11	1:A:305:LEU:HD12	1.83	0.60
1:C:191:LEU:O	1:C:192:VAL:CG2	2.50	0.60
1:D:75:LEU:HD22	1:D:213:LEU:HD11	1.84	0.60
1:D:167:ILE:HD12	1:D:167:ILE:N	2.16	0.60
1:D:277:LEU:HD23	1:D:301:ASP:HB3	1.84	0.60
1:B:63:ASN:HD22	1:B:65:SER:H	1.50	0.60
1:B:93:GLN:HG2	1:B:97:GLN:OE1	2.02	0.59
1:C:280:CYS:SG	1:C:289:GLU:HB2	2.41	0.59
1:D:414:PRO:O	1:D:415:LEU:HD12	2.02	0.59
1:D:419:VAL:HA	1:D:441:HIS:O	2.01	0.59
1:A:48:ARG:NH1	1:A:87:GLU:HG3	2.16	0.59
1:A:176:LEU:CD2	1:A:350:GLN:HG3	2.32	0.59
1:B:478:LEU:O	1:B:480:PRO:HD3	2.02	0.59
1:D:98:SER:O	1:D:193:PRO:HD2	2.03	0.59
1:D:237:GLY:H	1:D:243:PRO:HA	1.67	0.59
1:C:160:SER:HA	1:C:417:LEU:HD13	1.84	0.59
1:B:317:SER:OG	1:B:319:HIS:HD2	1.85	0.59
1:C:33:PRO:O	1:C:34:LYS:CG	2.50	0.59
1:C:79:ARG:HG3	1:C:207:THR:HG22	1.84	0.59
1:A:154:THR:HA	1:A:157:LYS:HD2	1.83	0.59
1:B:408:ARG:CG	1:B:408:ARG:O	2.51	0.59
1:D:368:ARG:O	1:D:370:GLN:N	2.35	0.59
1:B:431:LEU:HD23	1:B:432:ARG:N	2.17	0.59
1:D:442:ARG:HD2	1:D:445:PRO:O	2.01	0.59
1:A:291:LEU:HD11	1:A:360:LEU:HD22	1.84	0.59
1:B:279:ARG:NH2	1:B:426:ASP:OD2	2.35	0.59
1:B:128:VAL:O	1:B:131:PRO:HD2	2.03	0.59
1:C:180:ALA:HB2	1:C:345:ARG:O	2.02	0.59
1:C:390:GLU:CG	1:C:462:SER:HB3	2.32	0.59
1:B:265:ARG:HD2	1:B:316:LEU:HD12	1.85	0.58
1:B:427:VAL:HG12	1:B:467:PHE:CZ	2.38	0.58
1:C:116:HIS:CD2	1:C:218:ILE:HG23	2.38	0.58
1:C:191:LEU:C	1:C:192:VAL:HG22	2.28	0.58
1:D:276:PRO:HG2	1:D:397:LEU:CD2	2.33	0.58
1:D:353:ASP:OD2	1:D:355:GLY:N	2.30	0.58
1:D:215:THR:HA	1:D:255:LEU:HD21	1.84	0.58
1:A:192:VAL:N	1:A:193:PRO:HD3	2.17	0.58
1:B:278:GLY:HA3	1:B:289:GLU:OE2	2.04	0.58
1:D:211:LEU:HG	1:D:251:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLN:NE2	1:A:101:GLN:N	2.51	0.58
1:C:230:LEU:C	1:C:230:LEU:HD13	2.28	0.58
1:D:424:LEU:HD12	1:D:436:PRO:C	2.28	0.58
1:C:281:VAL:HB	1:C:421:ALA:HB3	1.85	0.58
1:D:54:ILE:HG21	1:D:90:VAL:HG12	1.86	0.58
1:A:108:TRP:N	1:A:108:TRP:CD1	2.71	0.58
1:B:63:ASN:C	1:B:63:ASN:ND2	2.56	0.58
1:C:84:ASP:OD1	1:C:87:GLU:HG3	2.03	0.58
1:D:431:LEU:HD23	1:D:431:LEU:H	1.67	0.58
1:C:93:GLN:O	1:C:97:GLN:HG3	2.03	0.58
1:C:340:LEU:HD22	1:C:340:LEU:O	2.03	0.58
1:C:386:ASP:OD1	1:C:386:ASP:C	2.45	0.58
1:C:364:SER:O	1:C:367:GLU:N	2.36	0.58
1:D:371:LEU:HD12	1:D:371:LEU:N	2.18	0.58
1:B:56:GLY:O	1:B:59:ALA:HB3	2.03	0.58
1:C:249:ARG:HG2	1:C:249:ARG:HH11	1.67	0.58
1:C:464:ARG:HH11	1:C:464:ARG:CB	2.17	0.58
1:D:478:LEU:HB3	1:D:479:PRO:HD2	1.85	0.58
1:C:106:GLU:OE2	1:C:106:GLU:HA	2.03	0.57
1:D:387:GLY:O	1:D:430:ARG:HG3	2.03	0.57
1:A:244:ASN:ND2	1:A:245:GLN:NE2	2.51	0.57
1:D:230:LEU:HD11	1:D:232:VAL:HG22	1.86	0.57
1:A:283:HIS:O	1:A:287:VAL:HG23	2.04	0.57
1:B:340:LEU:HD22	1:B:361:CYS:HB3	1.85	0.57
1:D:270:LEU:O	1:D:271:THR:HG23	2.04	0.57
1:A:384:PRO:HD3	1:A:456:GLN:HE22	1.70	0.57
1:D:124:LYS:HE3	1:D:289:GLU:OE2	2.04	0.57
1:D:322:THR:HG23	1:D:325:GLN:N	2.11	0.57
1:B:83:MET:HE2	1:B:87:GLU:CB	2.34	0.57
1:B:367:GLU:O	1:B:371:LEU:HD13	2.05	0.57
1:C:230:LEU:HD11	1:C:232:VAL:CG2	2.33	0.57
1:D:113:VAL:HG12	1:D:229:ALA:HB3	1.86	0.57
1:D:404:LEU:O	1:D:419:VAL:HG21	2.03	0.57
1:B:419:VAL:HA	1:B:441:HIS:O	2.04	0.57
1:C:146:ARG:NH1	1:C:156:ASP:OD2	2.38	0.57
1:B:61:VAL:HG12	1:B:197:ILE:HD12	1.86	0.57
1:D:79:ARG:HG3	1:D:207:THR:HG22	1.87	0.57
1:D:245:GLN:CD	1:D:245:GLN:N	2.62	0.56
1:D:264:LEU:HB3	1:D:266:VAL:HG23	1.87	0.56
1:D:356:LEU:HD13	1:D:356:LEU:C	2.30	0.56
1:B:114:ASP:HB3	1:B:227:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ALA:O	1:B:135:ALA:HB3	2.05	0.56
1:A:244:ASN:HD22	1:A:245:GLN:N	2.02	0.56
1:B:115:LYS:HA	1:B:231:VAL:O	2.05	0.56
1:B:244:ASN:ND2	1:B:245:GLN:H	2.02	0.56
1:C:211:LEU:N	1:C:212:PRO:HD2	2.20	0.56
1:C:239:ALA:HB3	1:C:273:MET:O	2.06	0.56
1:A:63:ASN:C	1:A:63:ASN:ND2	2.61	0.56
1:B:139:LYS:HE3	1:B:177:LEU:HB3	1.88	0.56
1:C:38:GLU:O	1:C:42:MET:HG3	2.06	0.56
1:D:211:LEU:HD21	1:D:254:THR:HG21	1.88	0.56
1:D:353:ASP:OD2	1:D:354:PRO:N	2.38	0.56
1:A:244:ASN:HB3	1:A:247:GLN:HB3	1.88	0.56
1:B:168:GLN:CG	1:B:185:VAL:HG11	2.36	0.56
1:C:111:GLN:O	1:C:139:LYS:HB2	2.06	0.56
1:C:364:SER:H	1:C:367:GLU:HG2	1.71	0.56
1:A:459:LEU:HD13	1:A:460:VAL:N	2.21	0.56
1:C:353:ASP:O	1:C:356:LEU:N	2.38	0.56
1:C:384:PRO:O	1:C:433:ARG:HG3	2.05	0.56
1:B:148:LEU:HD13	1:B:199:TYR:CE1	2.41	0.56
1:C:305:LEU:HD13	1:C:309:LEU:HD12	1.87	0.56
1:B:134:ALA:HA	1:B:138:CYS:O	2.06	0.55
1:D:122:GLY:HA2	1:D:286:GLU:OE2	2.06	0.55
1:D:305:LEU:HD23	1:D:472:PRO:HG2	1.86	0.55
1:D:223:LEU:CD1	1:D:262:LEU:HD13	2.35	0.55
1:D:376:ARG:HD3	1:D:443:ASP:O	2.06	0.55
1:D:387:GLY:C	1:D:430:ARG:HG3	2.32	0.55
1:C:291:LEU:CD1	1:C:368:ARG:HD3	2.36	0.55
1:D:251:LEU:C	1:D:251:LEU:HD13	2.32	0.55
1:B:120:GLY:HA2	1:B:273:MET:SD	2.47	0.55
1:B:413:GLU:HB2	1:B:414:PRO:HD2	1.88	0.55
1:D:476:LEU:HD21	1:D:478:LEU:HD21	1.88	0.55
1:B:428:GLY:HA3	1:B:467:PHE:O	2.06	0.55
1:C:136:CYS:SG	1:C:329:ARG:HD2	2.46	0.55
1:C:385:ALA:O	1:C:386:ASP:C	2.47	0.55
1:D:63:ASN:N	1:D:63:ASN:HD22	2.05	0.55
1:C:117:SER:HA	1:C:233:ASP:HB3	1.88	0.55
1:D:113:VAL:O	1:D:114:ASP:HB2	2.06	0.55
1:A:131:PRO:HG2	1:A:294:MET:HE1	1.89	0.55
1:C:79:ARG:HG3	1:C:207:THR:HA	1.89	0.55
1:C:134:ALA:HB2	1:C:182:CYS:HB3	1.88	0.55
1:C:416:ARG:HG2	1:C:443:ASP:OD1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:GLY:O	1:D:286:GLU:HG3	2.07	0.55
1:A:374:ARG:HH21	1:A:374:ARG:HG2	1.72	0.55
1:C:440:VAL:HG11	1:C:447:LEU:HD11	1.88	0.55
1:A:104:TRP:O	1:A:109:ARG:NH1	2.39	0.55
1:B:79:ARG:NH1	1:B:209:ASP:OD2	2.40	0.55
1:B:391:LEU:HD21	1:B:393:ARG:HH11	1.72	0.55
1:A:246:GLU:C	1:A:248:ALA:H	2.14	0.54
1:A:316:LEU:C	1:A:318:GLY:H	2.16	0.54
1:B:43:LYS:HG3	1:B:74:MET:HE1	1.89	0.54
1:B:230:LEU:HD22	1:B:231:VAL:N	2.22	0.54
1:D:211:LEU:HD23	1:D:211:LEU:C	2.32	0.54
1:D:279:ARG:HD3	1:D:426:ASP:OD1	2.06	0.54
1:A:211:LEU:N	1:A:212:PRO:HD2	2.22	0.54
1:A:205:THR:HG22	1:A:205:THR:O	2.08	0.54
1:D:356:LEU:CD2	1:D:371:LEU:HD23	2.32	0.54
1:B:271:THR:HG22	1:B:473:PHE:HA	1.90	0.54
1:B:408:ARG:HB2	1:B:415:LEU:HD12	1.90	0.54
1:C:393:ARG:HG2	1:C:393:ARG:NH1	2.23	0.54
1:A:231:VAL:HG23	1:A:313:LEU:CD2	2.37	0.54
1:B:146:ARG:C	1:B:153:GLY:HA3	2.33	0.54
1:B:219:LEU:O	1:B:223:LEU:HB2	2.08	0.54
1:C:205:THR:O	1:C:206:ALA:HB3	2.07	0.54
1:C:155:LEU:O	1:C:159:GLU:HG2	2.08	0.54
1:C:284:ALA:O	1:C:288:GLU:HG3	2.07	0.54
1:C:214:ILE:HG23	1:C:218:ILE:HD12	1.90	0.54
1:C:205:THR:HG22	1:C:207:THR:HG23	1.90	0.53
1:D:108:TRP:O	1:D:112:LEU:HG	2.08	0.53
1:A:285:LEU:HD21	1:A:441:HIS:HD2	1.73	0.53
1:B:244:ASN:ND2	1:B:245:GLN:N	2.56	0.53
1:C:244:ASN:HB3	1:C:247:GLN:HB3	1.89	0.53
1:C:312:ALA:HB2	1:C:323:GLN:OE1	2.08	0.53
1:D:163:GLY:HA3	1:D:352:VAL:HA	1.91	0.53
1:D:271:THR:HG22	1:D:473:PHE:HA	1.90	0.53
1:B:32:GLU:O	1:B:32:GLU:HG3	2.08	0.53
1:B:408:ARG:CB	1:B:415:LEU:CD1	2.86	0.53
1:D:75:LEU:HD13	1:D:202:ARG:HG3	1.90	0.53
1:D:76:MET:CE	1:D:79:ARG:HB3	2.37	0.53
1:C:442:ARG:HG2	1:C:447:LEU:HD21	1.90	0.53
1:D:95:LEU:HD13	1:D:195:ASP:HB2	1.89	0.53
1:B:223:LEU:HD11	1:B:262:LEU:HD13	1.90	0.53
1:C:364:SER:H	1:C:367:GLU:CG	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ARG:O	1:D:252:ALA:HB3	2.08	0.53
1:A:184:ILE:H	1:A:350:GLN:HE22	1.57	0.53
1:A:191:LEU:C	1:A:193:PRO:HD3	2.33	0.53
1:C:148:LEU:HD13	1:C:199:TYR:CE1	2.44	0.53
1:C:381:LEU:O	1:C:382:LEU:C	2.52	0.53
1:D:57:PHE:CZ	1:D:74:MET:HG2	2.44	0.53
1:D:173:MET:HE3	1:D:183:CYS:SG	2.48	0.53
1:A:331:ALA:O	1:A:334:LEU:HB2	2.08	0.53
1:A:459:LEU:HD13	1:A:459:LEU:C	2.33	0.53
1:B:229:ALA:HB1	1:B:316:LEU:HB3	1.89	0.53
1:B:239:ALA:HB3	1:B:273:MET:O	2.09	0.53
1:C:131:PRO:HG2	1:C:294:MET:HE1	1.89	0.53
1:C:160:SER:CA	1:C:417:LEU:HD13	2.38	0.53
1:A:322:THR:HG23	1:A:325:GLN:H	1.73	0.53
1:B:143:ILE:HA	1:B:185:VAL:O	2.07	0.53
1:C:388:THR:HA	1:C:430:ARG:HB3	1.91	0.53
1:D:121:VAL:HG23	1:D:239:ALA:HB1	1.89	0.53
1:C:431:LEU:HD12	1:C:435:THR:HB	1.91	0.53
1:D:114:ASP:OD2	1:D:115:LYS:N	2.42	0.53
1:B:50:SER:C	1:B:52:ALA:N	2.65	0.52
1:C:295:ASP:O	1:C:296:GLY:C	2.51	0.52
1:B:128:VAL:HA	1:B:294:MET:HE3	1.90	0.52
1:C:170:PRO:HA	1:C:173:MET:CE	2.34	0.52
1:C:188:SER:C	1:C:190:GLN:H	2.17	0.52
1:D:36:LEU:HD23	1:D:70:GLN:CD	2.35	0.52
1:D:141:PRO:HA	1:D:183:CYS:HG	1.73	0.52
1:A:92:THR:HG23	1:A:93:GLN:H	1.75	0.52
1:B:249:ARG:HG2	1:B:270:LEU:HD11	1.91	0.52
1:C:134:ALA:HA	1:C:138:CYS:O	2.09	0.52
1:C:386:ASP:OD1	1:C:387:GLY:N	2.43	0.52
1:A:384:PRO:HD3	1:A:456:GLN:NE2	2.24	0.52
1:B:278:GLY:HA2	1:B:299:PRO:CB	2.40	0.52
1:B:356:LEU:HD12	1:B:360:LEU:HD12	1.90	0.52
1:C:274:ASP:O	1:C:394:ALA:CB	2.55	0.52
1:D:130:ALA:CB	1:D:131:PRO:HD3	2.31	0.52
1:B:377:GLU:HB3	1:B:442:ARG:NH2	2.22	0.52
1:C:156:ASP:HA	1:C:159:GLU:HG3	1.90	0.52
1:C:393:ARG:O	1:C:396:PRO:HD2	2.10	0.52
1:D:202:ARG:O	1:D:208:VAL:HG23	2.10	0.52
1:D:333:ALA:HA	1:D:338:SER:HB2	1.90	0.52
1:A:246:GLU:C	1:A:248:ALA:N	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:O	1:B:295:ASP:HB2	2.10	0.52
1:C:36:LEU:HD11	1:C:66:ALA:HB2	1.92	0.52
1:C:76:MET:CE	1:C:80:LEU:HG	2.39	0.52
1:C:415:LEU:N	1:C:415:LEU:HD12	2.25	0.52
1:A:191:LEU:N	1:A:191:LEU:HD12	2.24	0.52
1:B:273:MET:HE1	1:B:276:PRO:HA	1.92	0.52
1:B:402:HIS:NE2	1:B:409:SER:CB	2.69	0.52
1:C:145:GLY:CA	1:C:155:LEU:HD12	2.40	0.52
1:C:229:ALA:CB	1:C:316:LEU:HD12	2.32	0.52
1:D:205:THR:O	1:D:206:ALA:CB	2.57	0.52
1:D:380:GLU:HG2	1:D:439:ARG:HD3	1.91	0.52
1:D:391:LEU:HD23	1:D:391:LEU:C	2.34	0.52
1:A:168:GLN:HG2	1:A:185:VAL:HG11	1.91	0.52
1:D:277:LEU:CD2	1:D:301:ASP:HB3	2.39	0.52
1:D:387:GLY:O	1:D:431:LEU:HD23	2.09	0.52
1:C:277:LEU:HD12	1:C:302:LEU:HD23	1.92	0.52
1:D:245:GLN:NE2	1:D:245:GLN:N	2.43	0.52
1:C:113:VAL:HA	1:C:229:ALA:O	2.09	0.51
1:C:329:ARG:O	1:C:332:ALA:HB3	2.10	0.51
1:D:289:GLU:HG2	1:D:302:LEU:HD11	1.92	0.51
1:D:388:THR:N	1:D:430:ARG:NH1	2.58	0.51
1:A:426:ASP:N	1:A:429:GLN:HE21	1.91	0.51
1:B:431:LEU:HD11	1:B:437:TRP:HB3	1.91	0.51
1:C:143:ILE:HG12	1:C:185:VAL:HG23	1.91	0.51
1:D:176:LEU:HD21	1:D:350:GLN:HE21	1.76	0.51
1:A:303:ARG:NH1	1:A:335:ASP:OD1	2.43	0.51
1:C:191:LEU:C	1:C:192:VAL:CG2	2.83	0.51
1:C:205:THR:O	1:C:205:THR:CG2	2.59	0.51
1:D:42:MET:HE1	1:D:53:ASP:OD2	2.10	0.51
1:C:247:GLN:C	1:C:249:ARG:H	2.18	0.51
1:B:83:MET:HB3	1:B:87:GLU:HB2	1.92	0.51
1:C:77:ALA:O	1:C:81:ARG:HB2	2.10	0.51
1:B:205:THR:O	1:B:205:THR:CG2	2.57	0.51
1:B:232:VAL:HG11	1:B:255:LEU:HD13	1.92	0.51
1:C:256:VAL:HG23	1:C:266:VAL:HG23	1.92	0.51
1:D:389:VAL:HG23	1:D:431:LEU:HD22	1.90	0.51
1:D:416:ARG:HH11	1:D:443:ASP:CG	2.14	0.51
1:B:172:GLN:O	1:B:175:VAL:HG12	2.10	0.51
1:B:285:LEU:CD2	1:B:369:ARG:HH21	2.21	0.51
1:C:76:MET:HE3	1:C:76:MET:O	2.11	0.51
1:C:191:LEU:O	1:C:192:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:THR:HG22	1:C:219:LEU:HD12	1.92	0.51
1:C:238:GLY:O	1:C:395:LEU:HD22	2.11	0.51
1:D:95:LEU:HD21	1:D:198:LEU:HD12	1.93	0.51
1:D:340:LEU:O	1:D:340:LEU:HD22	2.11	0.51
1:A:183:CYS:HB2	1:A:350:GLN:NE2	2.26	0.51
1:B:131:PRO:CB	1:B:294:MET:HE1	2.40	0.51
1:D:115:LYS:HD2	1:D:115:LYS:C	2.36	0.51
1:B:133:LEU:HD11	1:B:313:LEU:HD12	1.92	0.50
1:B:253:LYS:O	1:B:256:VAL:HG23	2.11	0.50
1:C:34:LYS:NZ	1:C:42:MET:HE1	2.27	0.50
1:C:205:THR:O	1:C:205:THR:HG22	2.11	0.50
1:D:153:GLY:O	1:D:157:LYS:HG2	2.11	0.50
1:D:414:PRO:O	1:D:415:LEU:CD1	2.59	0.50
1:A:148:LEU:HD13	1:A:199:TYR:CE1	2.47	0.50
1:C:74:MET:O	1:C:78:ILE:HG13	2.10	0.50
1:C:85:LEU:HD22	1:C:85:LEU:N	2.25	0.50
1:D:192:VAL:CG1	1:D:224:VAL:HG21	2.40	0.50
1:A:117:SER:HA	1:A:233:ASP:HB3	1.93	0.50
1:A:459:LEU:HD11	1:A:461:LEU:HG	1.93	0.50
1:B:84:ASP:OD2	1:B:87:GLU:HG3	2.10	0.50
1:B:205:THR:HG22	1:B:207:THR:HG23	1.93	0.50
1:B:304:ASP:OD1	1:B:472:PRO:HD2	2.12	0.50
1:D:353:ASP:C	1:D:353:ASP:OD2	2.55	0.50
1:A:244:ASN:HD22	1:A:244:ASN:C	2.19	0.50
1:A:364:SER:HB3	1:C:97:GLN:O	2.10	0.50
1:C:156:ASP:OD2	1:C:408:ARG:NH2	2.44	0.50
1:C:276:PRO:HD3	1:C:394:ALA:HB2	1.92	0.50
1:D:244:ASN:HD22	1:D:244:ASN:C	2.19	0.50
1:B:50:SER:C	1:B:52:ALA:H	2.19	0.50
1:B:245:GLN:O	1:B:249:ARG:HG3	2.11	0.50
1:B:252:ALA:O	1:B:256:VAL:HG22	2.11	0.50
1:B:378:GLN:HE21	1:B:439:ARG:HD3	1.73	0.50
1:C:364:SER:N	1:C:367:GLU:HG2	2.26	0.50
1:D:413:GLU:O	1:D:414:PRO:O	2.30	0.50
1:B:124:LYS:H	1:B:124:LYS:HD2	1.77	0.50
1:B:166:VAL:HG23	1:B:167:ILE:CD1	2.40	0.50
1:B:195:ASP:OD1	1:B:221:LYS:HE3	2.11	0.50
1:D:369:ARG:O	1:D:374:ARG:HD3	2.12	0.50
1:A:215:THR:HG22	1:A:219:LEU:HD12	1.94	0.50
1:C:242:PHE:C	1:C:244:ASN:N	2.70	0.50
1:B:391:LEU:HD11	1:B:393:ARG:HH11	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:LEU:O	1:C:382:LEU:O	2.30	0.49
1:A:116:HIS:CD2	1:A:218:ILE:HG23	2.48	0.49
1:A:211:LEU:C	1:A:211:LEU:HD13	2.37	0.49
1:B:133:LEU:O	1:B:138:CYS:HB2	2.12	0.49
1:B:432:ARG:O	1:B:433:ARG:C	2.54	0.49
1:D:36:LEU:HB3	1:D:37:PRO:HD3	1.92	0.49
1:D:43:LYS:HG3	1:D:74:MET:CE	2.42	0.49
1:B:127:LEU:HD22	1:B:158:LEU:HD21	1.93	0.49
1:B:340:LEU:CD2	1:B:361:CYS:HB3	2.43	0.49
1:C:384:PRO:CD	1:C:459:LEU:HD13	2.42	0.49
1:D:367:GLU:O	1:D:370:GLN:HB2	2.12	0.49
1:D:431:LEU:HD23	1:D:431:LEU:N	2.26	0.49
1:C:125:VAL:HG13	1:C:306:VAL:CG2	2.42	0.49
1:C:148:LEU:HD13	1:C:199:TYR:CZ	2.48	0.49
1:D:291:LEU:O	1:D:295:ASP:HB2	2.12	0.49
1:B:118:THR:HG22	1:B:218:ILE:HD11	1.94	0.49
1:C:393:ARG:CG	1:C:396:PRO:HG2	2.40	0.49
1:A:173:MET:HA	1:A:176:LEU:HD12	1.94	0.49
1:B:139:LYS:HE3	1:B:177:LEU:O	2.13	0.49
1:B:231:VAL:HG23	1:B:313:LEU:HD23	1.93	0.49
1:B:442:ARG:HG3	1:B:442:ARG:NH2	2.27	0.49
1:D:76:MET:HE3	1:D:79:ARG:HB3	1.94	0.49
1:D:363:GLY:O	1:D:364:SER:O	2.30	0.49
1:D:388:THR:HA	1:D:430:ARG:HA	1.94	0.49
1:A:393:ARG:HG2	1:A:393:ARG:HH11	1.76	0.49
1:B:51:GLU:HA	1:B:90:VAL:HG11	1.95	0.49
1:C:36:LEU:HB2	1:C:37:PRO:HD3	1.94	0.49
1:C:291:LEU:HD13	1:C:368:ARG:HD3	1.95	0.49
1:C:379:GLU:HG2	1:C:442:ARG:HD3	1.94	0.49
1:D:321:GLY:H	1:D:325:GLN:NE2	2.11	0.49
1:B:290:ALA:O	1:B:294:MET:HG3	2.13	0.49
1:C:211:LEU:HD21	1:C:251:LEU:HA	1.93	0.49
1:C:292:LEU:HD11	1:C:365:PRO:CG	2.43	0.49
1:C:386:ASP:H	1:C:433:ARG:HB2	1.76	0.49
1:D:180:ALA:O	1:D:342:ARG:HG3	2.13	0.49
1:D:236:PHE:CE2	1:D:474:ALA:HB2	2.47	0.49
1:C:275:LYS:HD2	1:C:427:VAL:HG21	1.94	0.49
1:D:388:THR:OG1	1:D:430:ARG:NH1	2.46	0.49
1:A:190:GLN:HB2	1:A:191:LEU:HD12	1.95	0.49
1:D:365:PRO:O	1:D:367:GLU:N	2.46	0.49
1:D:376:ARG:NH1	1:D:377:GLU:HB2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:SER:C	1:A:212:PRO:HD2	2.38	0.48
1:A:279:ARG:H	1:A:289:GLU:CD	2.20	0.48
1:B:379:GLU:HG2	1:B:442:ARG:HH11	1.78	0.48
1:C:112:LEU:HD23	1:C:139:LYS:O	2.13	0.48
1:C:234:VAL:HG11	1:C:248:ALA:O	2.14	0.48
1:D:365:PRO:O	1:D:368:ARG:HB2	2.12	0.48
1:A:245:GLN:CD	1:A:245:GLN:H	2.21	0.48
1:A:249:ARG:HG3	1:A:270:LEU:HD11	1.94	0.48
1:B:89:SER:C	1:B:92:THR:HG22	2.39	0.48
1:B:253:LYS:HA	1:B:256:VAL:CG2	2.43	0.48
1:C:192:VAL:N	1:C:193:PRO:HD3	2.28	0.48
1:C:352:VAL:HG12	1:C:353:ASP:N	2.28	0.48
1:D:205:THR:HG22	1:D:207:THR:HG23	1.94	0.48
1:C:133:LEU:CD1	1:C:313:LEU:HD12	2.42	0.48
1:C:437:TRP:CE2	1:C:459:LEU:HD12	2.48	0.48
1:B:114:ASP:HB3	1:B:227:LEU:CD1	2.43	0.48
1:B:231:VAL:HG23	1:B:313:LEU:CD2	2.43	0.48
1:A:244:ASN:ND2	1:A:244:ASN:C	2.70	0.48
1:A:370:GLN:HA	1:A:374:ARG:CZ	2.43	0.48
1:B:101:GLN:HE22	1:B:224:VAL:HG23	1.78	0.48
1:D:157:LYS:HE3	1:D:286:GLU:CD	2.38	0.48
1:D:281:VAL:HA	1:D:286:GLU:OE2	2.14	0.48
1:D:381:LEU:HD23	1:D:438:LEU:HD23	1.96	0.48
1:B:279:ARG:HH21	1:B:426:ASP:CG	2.21	0.48
1:B:379:GLU:CD	1:B:442:ARG:HE	2.21	0.48
1:D:36:LEU:HD11	1:D:57:PHE:CD1	2.43	0.48
1:D:161:ILE:HD12	1:D:360:LEU:HD21	1.95	0.48
1:D:172:GLN:O	1:D:176:LEU:HD13	2.13	0.48
1:D:367:GLU:OE2	1:D:367:GLU:HA	2.13	0.48
1:A:54:ILE:O	1:A:58:VAL:HG23	2.13	0.48
1:A:367:GLU:C	1:A:371:LEU:HD12	2.38	0.48
1:A:118:THR:HG23	1:A:233:ASP:O	2.14	0.48
1:A:432:ARG:O	1:A:435:THR:HG23	2.13	0.48
1:C:113:VAL:O	1:C:114:ASP:HB2	2.12	0.48
1:C:265:ARG:HD2	1:C:316:LEU:CD1	2.43	0.48
1:D:201:ALA:O	1:D:202:ARG:C	2.57	0.48
1:A:79:ARG:HD3	1:A:79:ARG:C	2.37	0.48
1:A:104:TRP:N	1:A:109:ARG:HH12	2.06	0.48
1:A:158:LEU:HD13	1:A:164:PHE:CZ	2.49	0.48
1:B:323:GLN:O	1:B:327:ALA:N	2.37	0.48
1:C:188:SER:O	1:C:193:PRO:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ASN:ND2	1:D:65:SER:H	2.12	0.48
1:D:387:GLY:C	1:D:430:ARG:HH11	2.22	0.48
1:A:390:GLU:CD	1:A:464:ARG:HH21	2.22	0.48
1:C:128:VAL:O	1:C:131:PRO:HD2	2.14	0.48
1:A:168:GLN:HG2	1:A:185:VAL:CG1	2.44	0.47
1:C:235:LYS:HE3	1:C:273:MET:CG	2.43	0.47
1:D:158:LEU:HD13	1:D:164:PHE:CZ	2.49	0.47
1:D:284:ALA:O	1:D:288:GLU:HG3	2.14	0.47
1:A:89:SER:O	1:A:92:THR:HG23	2.13	0.47
1:A:241:VAL:O	1:A:243:PRO:HD3	2.14	0.47
1:B:158:LEU:C	1:B:160:SER:H	2.21	0.47
1:B:174:GLN:HG3	1:B:175:VAL:N	2.28	0.47
1:B:265:ARG:HD2	1:B:316:LEU:CD1	2.44	0.47
1:C:230:LEU:HD11	1:C:232:VAL:HG23	1.96	0.47
1:D:60:ALA:HB1	1:D:66:ALA:HB2	1.96	0.47
1:D:244:ASN:HB3	1:D:247:GLN:CB	2.42	0.47
1:D:356:LEU:HD21	1:D:371:LEU:HB3	1.95	0.47
1:A:165:ASN:HB3	1:A:168:GLN:NE2	2.26	0.47
1:A:244:ASN:HD21	1:A:245:GLN:NE2	2.11	0.47
1:A:382:LEU:HD22	1:A:434:GLY:O	2.14	0.47
1:C:141:PRO:O	1:C:225:GLU:CD	2.57	0.47
1:D:402:HIS:ND1	1:D:407:GLY:HA3	2.30	0.47
1:A:219:LEU:O	1:A:223:LEU:HG	2.14	0.47
1:A:252:ALA:O	1:A:256:VAL:HG23	2.15	0.47
1:B:175:VAL:CG1	1:B:176:LEU:N	2.77	0.47
1:A:106:GLU:O	1:A:109:ARG:HB2	2.14	0.47
1:B:379:GLU:HG2	1:B:442:ARG:NH1	2.29	0.47
1:C:438:LEU:HG	1:C:439:ARG:N	2.29	0.47
1:B:204:VAL:HG12	1:B:409:SER:HA	1.95	0.47
1:D:192:VAL:HG21	1:D:221:LYS:HG2	1.96	0.47
1:A:367:GLU:O	1:A:371:LEU:HD12	2.15	0.47
1:A:390:GLU:O	1:A:427:VAL:HG13	2.14	0.47
1:A:445:PRO:O	1:A:446:ALA:CB	2.59	0.47
1:B:34:LYS:HE3	1:B:42:MET:CE	2.44	0.47
1:C:348:ALA:HB1	1:C:354:PRO:HG3	1.96	0.47
1:C:463:ASP:OD2	1:C:463:ASP:N	2.46	0.47
1:D:92:THR:HG22	1:D:216:ALA:HA	1.96	0.47
1:D:118:THR:HG1	1:D:235:LYS:H	1.62	0.47
1:D:285:LEU:HD11	1:D:441:HIS:HD2	1.80	0.47
1:A:83:MET:HE2	1:A:212:PRO:HB2	1.97	0.47
1:C:119:GLY:O	1:C:235:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ILE:HA	1:C:185:VAL:O	2.15	0.47
1:D:148:LEU:HD13	1:D:199:TYR:CZ	2.50	0.47
1:B:460:VAL:O	1:B:461:LEU:HD23	2.14	0.47
1:C:192:VAL:HG13	1:C:224:VAL:HG21	1.96	0.47
1:C:299:PRO:HA	1:C:300:PRO:HD3	1.79	0.47
1:C:307:THR:HA	1:C:330:VAL:HG11	1.97	0.47
1:A:391:LEU:HD23	1:A:460:VAL:CG2	2.44	0.47
1:B:148:LEU:HD21	1:B:202:ARG:CZ	2.45	0.47
1:B:244:ASN:HD22	1:B:245:GLN:H	1.62	0.47
1:B:333:ALA:HB1	1:B:339:ALA:HB2	1.96	0.47
1:C:319:HIS:N	1:C:319:HIS:CD2	2.83	0.47
1:C:367:GLU:O	1:C:371:LEU:HD13	2.15	0.47
1:C:384:PRO:HG2	1:C:385:ALA:H	1.80	0.47
1:C:424:LEU:O	1:C:425:VAL:HG13	2.15	0.47
1:D:468:ALA:O	1:D:469:ALA:C	2.57	0.47
1:A:129:LEU:HD21	1:A:310:GLY:HA2	1.98	0.46
1:B:74:MET:HE2	1:B:78:ILE:HG13	1.96	0.46
1:C:84:ASP:CG	1:C:87:GLU:HG3	2.41	0.46
1:C:453:ARG:NH1	1:C:453:ARG:CB	2.74	0.46
1:D:276:PRO:CG	1:D:397:LEU:HD23	2.44	0.46
1:A:232:VAL:HG11	1:A:255:LEU:HD12	1.97	0.46
1:B:39:LEU:HD22	1:B:53:ASP:HB3	1.96	0.46
1:B:249:ARG:O	1:B:252:ALA:HB3	2.15	0.46
1:C:125:VAL:HG13	1:C:306:VAL:HG22	1.96	0.46
1:C:305:LEU:HD13	1:C:309:LEU:CD1	2.45	0.46
1:C:390:GLU:HB2	1:C:460:VAL:O	2.15	0.46
1:C:473:PHE:HZ	1:C:476:LEU:HB2	1.80	0.46
1:C:478:LEU:CG	1:C:479:PRO:HD2	2.45	0.46
1:D:296:GLY:O	1:D:297:ALA:HB2	2.15	0.46
1:D:383:ALA:HB2	1:D:431:LEU:HD12	1.97	0.46
1:D:430:ARG:HG3	1:D:430:ARG:HH11	1.81	0.46
1:A:236:PHE:CD1	1:A:236:PHE:C	2.94	0.46
1:A:80:LEU:O	1:A:81:ARG:HD2	2.15	0.46
1:C:236:PHE:CD1	1:C:236:PHE:O	2.69	0.46
1:D:38:GLU:O	1:D:42:MET:HG3	2.15	0.46
1:D:111:GLN:O	1:D:139:LYS:N	2.47	0.46
1:A:205:THR:CG2	1:A:207:THR:OG1	2.63	0.46
1:C:214:ILE:HD13	1:C:214:ILE:HA	1.86	0.46
1:C:388:THR:HA	1:C:430:ARG:HB2	1.96	0.46
1:D:60:ALA:CB	1:D:66:ALA:HB2	2.46	0.46
1:A:459:LEU:CD1	1:A:459:LEU:C	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:LEU:HB3	1:B:352:VAL:HG21	1.97	0.46
1:C:451:GLN:O	1:C:452:SER:C	2.57	0.46
1:D:96:ALA:C	1:D:101:GLN:HE22	2.16	0.46
1:D:345:ARG:O	1:D:349:ALA:HB2	2.16	0.46
1:D:455:LEU:O	1:D:458:ALA:HB3	2.15	0.46
1:C:347:LEU:O	1:C:352:VAL:HG23	2.16	0.46
1:A:106:GLU:HA	1:A:109:ARG:HD3	1.98	0.46
1:A:292:LEU:HD22	1:A:298:GLY:CA	2.45	0.46
1:B:84:ASP:OD2	1:B:84:ASP:C	2.59	0.46
1:C:43:LYS:HE3	1:C:43:LYS:HA	1.98	0.46
1:C:437:TRP:NE1	1:C:459:LEU:HD12	2.30	0.46
1:D:233:ASP:OD1	1:D:271:THR:OG1	2.33	0.46
1:A:146:ARG:NH1	1:A:156:ASP:OD2	2.44	0.46
1:B:134:ALA:HB2	1:B:182:CYS:HB3	1.98	0.46
1:B:246:GLU:HA	1:B:249:ARG:HD3	1.97	0.46
1:C:242:PHE:O	1:C:244:ASN:N	2.48	0.46
1:C:402:HIS:C	1:C:404:LEU:H	2.23	0.46
1:D:215:THR:HG23	1:D:255:LEU:HD23	1.97	0.46
1:C:83:MET:HB2	1:C:87:GLU:OE2	2.16	0.46
1:C:419:VAL:HG12	1:C:420:GLY:N	2.31	0.46
1:D:363:GLY:C	1:D:368:ARG:NH1	2.60	0.46
1:A:108:TRP:O	1:A:109:ARG:C	2.59	0.45
1:C:424:LEU:HB2	1:C:437:TRP:C	2.41	0.45
1:D:75:LEU:HD13	1:D:202:ARG:CG	2.46	0.45
1:B:89:SER:HA	1:B:92:THR:HG22	1.97	0.45
1:B:408:ARG:CB	1:B:415:LEU:HD12	2.45	0.45
1:C:76:MET:HE2	1:C:80:LEU:CD1	2.45	0.45
1:C:143:ILE:HG12	1:C:185:VAL:CG2	2.45	0.45
1:A:153:GLY:O	1:A:157:LYS:HG3	2.17	0.45
1:B:202:ARG:HA	1:B:207:THR:OG1	2.15	0.45
1:C:135:ALA:HA	1:C:342:ARG:HH11	1.78	0.45
1:C:265:ARG:CB	1:C:265:ARG:HH11	2.28	0.45
1:C:416:ARG:HB2	1:C:419:VAL:HG23	1.97	0.45
1:D:307:THR:HA	1:D:330:VAL:HG11	1.97	0.45
1:D:422:GLU:O	1:D:438:LEU:HD12	2.16	0.45
1:B:146:ARG:HG2	1:B:146:ARG:HH11	1.81	0.45
1:B:352:VAL:HG12	1:B:356:LEU:HB3	1.98	0.45
1:C:83:MET:CB	1:C:87:GLU:CD	2.90	0.45
1:D:425:VAL:HG11	1:D:431:LEU:HD13	1.98	0.45
1:A:393:ARG:HB3	1:A:396:PRO:HD2	1.98	0.45
1:C:36:LEU:N	1:C:37:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLN:O	1:C:101:GLN:NE2	2.50	0.45
1:C:333:ALA:HA	1:C:336:ASP:OD2	2.17	0.45
1:C:431:LEU:HD21	1:C:461:LEU:HD21	1.97	0.45
1:A:34:LYS:HD2	1:A:39:LEU:CD2	2.47	0.45
1:A:135:ALA:HB1	1:A:338:SER:HB3	1.98	0.45
1:A:373:PRO:O	1:A:418:GLY:HA2	2.17	0.45
1:B:378:GLN:HB2	1:B:440:VAL:O	2.17	0.45
1:C:279:ARG:HG2	1:C:279:ARG:NH2	2.31	0.45
1:C:344:GLU:HB2	1:C:361:CYS:SG	2.56	0.45
1:D:80:LEU:C	1:D:81:ARG:HG2	2.42	0.45
1:D:211:LEU:HD23	1:D:212:PRO:N	2.32	0.45
1:A:98:SER:OG	1:A:193:PRO:HD2	2.17	0.45
1:A:101:GLN:NE2	1:A:101:GLN:H	2.14	0.45
1:A:205:THR:O	1:A:206:ALA:HB3	2.16	0.45
1:B:256:VAL:HA	1:B:266:VAL:HB	1.98	0.45
1:B:285:LEU:HD21	1:B:369:ARG:HH22	1.76	0.45
1:B:341:GLY:O	1:B:342:ARG:C	2.60	0.45
1:C:276:PRO:CD	1:C:394:ALA:HB2	2.47	0.45
1:D:43:LYS:HB2	1:D:74:MET:HE1	1.99	0.45
1:A:48:ARG:NH1	1:A:84:ASP:OD2	2.50	0.45
1:A:382:LEU:CD2	1:A:436:PRO:HG3	2.47	0.45
1:B:50:SER:OG	1:B:52:ALA:HB3	2.16	0.45
1:B:191:LEU:O	1:B:192:VAL:C	2.60	0.45
1:C:342:ARG:HA	1:C:342:ARG:HD2	1.84	0.45
1:D:83:MET:HB2	1:D:87:GLU:HB2	1.99	0.45
1:D:365:PRO:C	1:D:367:GLU:N	2.75	0.45
1:A:54:ILE:HD12	1:A:90:VAL:HB	1.99	0.45
1:B:115:LYS:HG2	1:B:129:LEU:CD1	2.46	0.45
1:C:195:ASP:OD1	1:C:221:LYS:HE2	2.16	0.45
1:C:288:GLU:CG	1:C:372:LEU:HD12	2.47	0.45
1:D:43:LYS:CB	1:D:74:MET:HE1	2.47	0.45
1:D:367:GLU:CD	1:D:371:LEU:HD11	2.42	0.45
1:D:416:ARG:HB2	1:D:419:VAL:CG2	2.46	0.45
1:A:117:SER:OG	1:A:118:THR:N	2.50	0.45
1:B:249:ARG:CG	1:B:270:LEU:HD11	2.47	0.45
1:C:451:GLN:O	1:C:455:LEU:N	2.47	0.45
1:A:231:VAL:HG23	1:A:313:LEU:HD23	1.97	0.44
1:B:113:VAL:HB	1:B:313:LEU:HD22	1.99	0.44
1:B:127:LEU:CD2	1:B:158:LEU:HD21	2.47	0.44
1:C:188:SER:C	1:C:190:GLN:N	2.75	0.44
1:D:117:SER:HA	1:D:233:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ALA:HA	1:D:264:LEU:O	2.17	0.44
1:D:375:ALA:HB3	1:D:441:HIS:HB3	1.97	0.44
1:A:299:PRO:HA	1:A:300:PRO:HD3	1.86	0.44
1:B:86:GLU:O	1:B:90:VAL:HG23	2.17	0.44
1:C:85:LEU:N	1:C:85:LEU:CD2	2.79	0.44
1:C:164:PHE:CE2	1:C:347:LEU:HD23	2.53	0.44
1:C:294:MET:HE3	1:C:343:PHE:CG	2.52	0.44
1:D:176:LEU:HD23	1:D:183:CYS:HB2	1.99	0.44
1:A:230:LEU:HD12	1:A:266:VAL:HG22	1.99	0.44
1:B:167:ILE:HD12	1:B:167:ILE:N	2.32	0.44
1:B:201:ALA:O	1:B:202:ARG:C	2.61	0.44
1:C:102:LEU:HD13	1:C:104:TRP:CZ2	2.53	0.44
1:C:235:LYS:HE3	1:C:273:MET:HG3	1.99	0.44
1:D:76:MET:HE3	1:D:79:ARG:CB	2.46	0.44
1:A:169:SER:O	1:A:170:PRO:C	2.58	0.44
1:A:432:ARG:HD3	1:A:432:ARG:N	2.31	0.44
1:B:113:VAL:O	1:B:114:ASP:HB2	2.16	0.44
1:B:304:ASP:OD1	1:B:471:SER:OG	2.28	0.44
1:B:390:GLU:O	1:B:391:LEU:HB3	2.17	0.44
1:A:48:ARG:HH12	1:A:87:GLU:HG3	1.79	0.44
1:A:122:GLY:O	1:A:124:LYS:NZ	2.41	0.44
1:A:191:LEU:O	1:A:192:VAL:C	2.61	0.44
1:A:202:ARG:CD	1:A:213:LEU:HD13	2.48	0.44
1:B:195:ASP:O	1:B:199:TYR:HB2	2.18	0.44
1:C:36:LEU:H	1:C:37:PRO:HD2	1.83	0.44
1:C:175:VAL:O	1:C:179:GLN:N	2.49	0.44
1:D:251:LEU:HD13	1:D:251:LEU:O	2.17	0.44
1:A:316:LEU:C	1:A:318:GLY:N	2.75	0.44
1:B:410:ARG:HA	1:B:410:ARG:HD3	1.64	0.44
1:C:279:ARG:HB3	1:C:423:LEU:HB2	1.99	0.44
1:C:376:ARG:HG3	1:C:443:ASP:OD2	2.16	0.44
1:C:379:GLU:OE1	1:C:442:ARG:HD3	2.18	0.44
1:C:476:LEU:HD23	1:C:476:LEU:C	2.42	0.44
1:D:291:LEU:O	1:D:295:ASP:N	2.50	0.44
1:A:476:LEU:O	1:A:478:LEU:HD12	2.17	0.44
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.78	0.44
1:C:46:GLY:HA2	1:C:81:ARG:HG3	1.98	0.44
1:C:160:SER:HA	1:C:417:LEU:CD1	2.47	0.44
1:C:215:THR:HG23	1:C:255:LEU:HD23	1.99	0.44
1:A:131:PRO:HG2	1:A:343:PHE:HD1	1.82	0.44
1:C:277:LEU:CD1	1:C:302:LEU:HD23	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:GLU:CA	1:D:109:ARG:HH11	2.29	0.44
1:D:148:LEU:HD13	1:D:199:TYR:CE1	2.52	0.44
1:A:410:ARG:O	1:A:411:ALA:C	2.61	0.44
1:B:246:GLU:O	1:B:250:GLU:HG2	2.18	0.44
1:C:82:GLY:C	1:C:83:MET:HG2	2.42	0.44
1:C:291:LEU:HD12	1:C:368:ARG:HD3	2.00	0.44
1:C:340:LEU:HD11	1:C:361:CYS:HB3	1.99	0.44
1:D:264:LEU:HB3	1:D:266:VAL:CG2	2.47	0.44
1:D:416:ARG:HD3	1:D:443:ASP:OD1	2.17	0.44
1:A:148:LEU:HD13	1:A:199:TYR:CZ	2.52	0.43
1:A:391:LEU:CD2	1:A:460:VAL:HG21	2.47	0.43
1:B:74:MET:HE3	1:B:74:MET:O	2.18	0.43
1:B:278:GLY:HA2	1:B:299:PRO:HB2	2.00	0.43
1:C:34:LYS:O	1:C:35:GLN:O	2.36	0.43
1:C:459:LEU:CD2	1:C:461:LEU:HG	2.42	0.43
1:D:105:PRO:O	1:D:106:GLU:C	2.61	0.43
1:D:146:ARG:HG2	1:D:155:LEU:HB2	1.99	0.43
1:A:265:ARG:HG2	1:A:316:LEU:HD11	1.99	0.43
1:B:311:GLY:C	1:B:323:GLN:HG3	2.43	0.43
1:C:364:SER:N	1:C:367:GLU:CG	2.81	0.43
1:A:118:THR:HG1	1:A:119:GLY:H	1.56	0.43
1:A:202:ARG:HD3	1:A:213:LEU:HD13	1.99	0.43
1:B:289:GLU:CD	1:B:299:PRO:HG2	2.43	0.43
1:C:211:LEU:HB3	1:C:212:PRO:HD3	2.01	0.43
1:D:211:LEU:N	1:D:212:PRO:HD2	2.33	0.43
1:A:320:ALA:O	1:A:321:GLY:C	2.61	0.43
1:A:389:VAL:HG12	1:A:427:VAL:HA	2.00	0.43
1:B:133:LEU:CD1	1:B:313:LEU:HD12	2.48	0.43
1:B:277:LEU:HD11	1:B:305:LEU:HD12	2.00	0.43
1:B:428:GLY:HA2	1:B:467:PHE:CD2	2.54	0.43
1:C:279:ARG:HH21	1:C:279:ARG:CG	2.31	0.43
1:C:401:LEU:HD13	1:C:404:LEU:CD1	2.44	0.43
1:D:63:ASN:ND2	1:D:63:ASN:H	2.16	0.43
1:D:79:ARG:HG3	1:D:207:THR:CA	2.41	0.43
1:B:381:LEU:CD1	1:B:438:LEU:HD23	2.35	0.43
1:B:383:ALA:CB	1:B:431:LEU:HD22	2.48	0.43
1:C:232:VAL:HG11	1:C:255:LEU:HD13	2.01	0.43
1:D:176:LEU:HD23	1:D:183:CYS:CB	2.48	0.43
1:A:269:ALA:HB2	1:A:476:LEU:CD1	2.45	0.43
1:A:308:THR:HG21	1:A:473:PHE:CD2	2.54	0.43
1:A:321:GLY:HA3	1:A:325:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:THR:O	1:A:389:VAL:C	2.61	0.43
1:B:48:ARG:NH1	1:B:87:GLU:HG2	2.34	0.43
1:B:79:ARG:HG3	1:B:207:THR:HA	1.99	0.43
1:B:129:LEU:HD22	1:B:133:LEU:CD1	2.48	0.43
1:B:141:PRO:O	1:B:225:GLU:OE1	2.36	0.43
1:B:192:VAL:N	1:B:193:PRO:HD3	2.34	0.43
1:C:48:ARG:CD	1:C:84:ASP:OD2	2.57	0.43
1:C:237:GLY:O	1:C:240:ALA:N	2.46	0.43
1:C:265:ARG:HH11	1:C:265:ARG:CG	2.31	0.43
1:D:424:LEU:CD1	1:D:436:PRO:HB2	2.48	0.43
1:A:130:ALA:HB3	1:A:131:PRO:CD	2.35	0.43
1:A:214:ILE:O	1:A:218:ILE:HG13	2.17	0.43
1:A:391:LEU:HA	1:A:427:VAL:CG2	2.46	0.43
1:B:222:LYS:HD3	1:B:222:LYS:HA	1.84	0.43
1:D:105:PRO:HD2	1:D:108:TRP:CE3	2.54	0.43
1:D:299:PRO:HD2	1:D:302:LEU:HD12	2.00	0.43
1:D:456:GLN:NE2	1:D:456:GLN:CA	2.75	0.43
1:A:83:MET:HB3	1:A:87:GLU:HB2	2.00	0.43
1:A:229:ALA:CB	1:A:316:LEU:HD12	2.38	0.43
1:A:439:ARG:HD2	1:A:441:HIS:CE1	2.53	0.43
1:B:43:LYS:CG	1:B:74:MET:HE1	2.47	0.43
1:C:111:GLN:HG3	1:C:319:HIS:HE1	1.83	0.43
1:C:184:ILE:H	1:C:350:GLN:HE22	1.66	0.43
1:D:86:GLU:O	1:D:87:GLU:C	2.62	0.43
1:D:115:LYS:HD2	1:D:116:HIS:N	2.33	0.43
1:D:124:LYS:H	1:D:124:LYS:HG2	1.49	0.43
1:D:211:LEU:HB3	1:D:212:PRO:CD	2.49	0.43
1:D:244:ASN:C	1:D:244:ASN:ND2	2.76	0.43
1:A:130:ALA:CB	1:A:131:PRO:HD3	2.36	0.43
1:C:142:MET:O	1:C:184:ILE:HA	2.19	0.43
1:D:275:LYS:HG3	1:D:276:PRO:O	2.19	0.43
1:C:49:LEU:HD12	1:C:49:LEU:HA	1.87	0.43
1:C:164:PHE:HE2	1:C:347:LEU:HD23	1.84	0.43
1:C:397:LEU:HD22	1:C:401:LEU:HD23	2.01	0.43
1:D:442:ARG:NH2	1:D:444:GLY:O	2.47	0.43
1:B:223:LEU:HA	1:B:264:LEU:HD11	2.00	0.42
1:C:247:GLN:C	1:C:249:ARG:N	2.75	0.42
1:A:176:LEU:HD22	1:A:350:GLN:HE21	1.84	0.42
1:A:268:ALA:O	1:A:477:VAL:N	2.52	0.42
1:B:382:LEU:HD22	1:B:434:GLY:O	2.19	0.42
1:C:462:SER:OG	1:C:463:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:ALA:HB1	1:B:438:LEU:HD11	2.01	0.42
1:C:106:GLU:OE2	1:C:109:ARG:HD3	2.19	0.42
1:C:356:LEU:O	1:C:359:ALA:HB3	2.19	0.42
1:C:386:ASP:CG	1:C:432:ARG:HA	2.42	0.42
1:C:442:ARG:H	1:C:442:ARG:HG3	1.64	0.42
1:A:104:TRP:O	1:A:105:PRO:C	2.60	0.42
1:A:202:ARG:HE	1:A:208:VAL:HA	1.84	0.42
1:B:49:LEU:HB2	1:B:54:ILE:HD13	2.01	0.42
1:B:166:VAL:O	1:B:185:VAL:HB	2.20	0.42
1:C:36:LEU:N	1:C:37:PRO:HD2	2.34	0.42
1:D:114:ASP:HB3	1:D:227:LEU:CD1	2.49	0.42
1:D:139:LYS:HA	1:D:181:GLY:O	2.20	0.42
1:D:146:ARG:C	1:D:153:GLY:HA3	2.45	0.42
1:A:63:ASN:HD21	1:A:65:SER:H	1.66	0.42
1:C:111:GLN:HG3	1:C:137:GLY:O	2.20	0.42
1:C:222:LYS:HA	1:C:222:LYS:HD3	1.82	0.42
1:D:57:PHE:CE2	1:D:74:MET:HG2	2.54	0.42
1:D:374:ARG:HG2	1:D:374:ARG:HH21	1.84	0.42
1:D:389:VAL:CG2	1:D:431:LEU:HD22	2.49	0.42
1:B:108:TRP:O	1:B:112:LEU:HG	2.19	0.42
1:B:324:ALA:O	1:B:325:GLN:C	2.59	0.42
1:C:83:MET:HB3	1:C:87:GLU:CD	2.44	0.42
1:C:211:LEU:HD13	1:C:211:LEU:C	2.45	0.42
1:C:237:GLY:O	1:C:238:GLY:C	2.62	0.42
1:A:158:LEU:C	1:A:160:SER:H	2.28	0.42
1:A:343:PHE:CZ	1:A:347:LEU:HD21	2.55	0.42
1:B:43:LYS:HB3	1:B:74:MET:HE1	2.02	0.42
1:C:79:ARG:CG	1:C:207:THR:HG22	2.49	0.42
1:C:177:LEU:O	1:C:181:GLY:HA2	2.20	0.42
1:D:43:LYS:HG3	1:D:74:MET:HE1	2.02	0.42
1:D:391:LEU:HG	1:D:392:VAL:N	2.34	0.42
1:A:94:ALA:O	1:A:95:LEU:C	2.63	0.42
1:A:108:TRP:CD1	1:A:108:TRP:H	2.37	0.42
1:A:238:GLY:HA3	1:A:274:ASP:HA	2.02	0.42
1:D:131:PRO:HB2	1:D:294:MET:CE	2.50	0.42
1:D:371:LEU:H	1:D:371:LEU:CD1	2.33	0.42
1:A:132:ALA:HB1	1:A:330:VAL:HG13	2.02	0.42
1:A:202:ARG:HD2	1:A:207:THR:O	2.19	0.42
1:A:292:LEU:HD22	1:A:298:GLY:HA2	2.01	0.42
1:B:89:SER:HA	1:B:92:THR:CG2	2.50	0.42
1:B:478:LEU:O	1:B:480:PRO:CD	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG21	1:A:98:SER:HB2	2.02	0.42
1:C:113:VAL:HG23	1:C:140:VAL:HG22	2.02	0.42
1:D:244:ASN:HD22	1:D:245:GLN:CD	2.28	0.42
1:D:424:LEU:HD12	1:D:436:PRO:HB2	2.02	0.42
1:B:210:SER:HB3	1:B:213:LEU:HB2	2.01	0.41
1:C:204:VAL:HG11	1:C:410:ARG:C	2.45	0.41
1:C:346:MET:O	1:C:346:MET:HG2	2.18	0.41
1:C:478:LEU:HD12	1:C:479:PRO:CD	2.42	0.41
1:D:164:PHE:HE2	1:D:346:MET:HE3	1.84	0.41
1:D:236:PHE:HE2	1:D:474:ALA:CB	2.33	0.41
1:A:381:LEU:N	1:A:381:LEU:CD2	2.83	0.41
1:B:120:GLY:HA2	1:B:273:MET:HG2	2.03	0.41
1:B:183:CYS:C	1:B:184:ILE:HG13	2.45	0.41
1:C:306:VAL:HG12	1:C:307:THR:N	2.36	0.41
1:D:130:ALA:HB3	1:D:131:PRO:CD	2.33	0.41
1:D:401:LEU:HD11	1:D:421:ALA:HB2	2.02	0.41
1:A:464:ARG:NH2	1:A:467:PHE:CZ	2.89	0.41
1:B:121:VAL:HG23	1:B:239:ALA:HB1	2.03	0.41
1:C:382:LEU:HD22	1:C:436:PRO:HG3	2.01	0.41
1:D:432:ARG:HH11	1:D:432:ARG:HG2	1.85	0.41
1:A:251:LEU:O	1:A:255:LEU:HG	2.20	0.41
1:B:148:LEU:HD13	1:B:199:TYR:CZ	2.55	0.41
1:C:400:VAL:C	1:C:402:HIS:N	2.76	0.41
1:D:36:LEU:HD23	1:D:70:GLN:OE1	2.20	0.41
1:D:230:LEU:HD13	1:D:230:LEU:C	2.46	0.41
1:A:231:VAL:HA	1:A:267:ALA:O	2.20	0.41
1:B:148:LEU:HD21	1:B:202:ARG:NH2	2.35	0.41
1:B:451:GLN:O	1:B:455:LEU:HG	2.21	0.41
1:C:237:GLY:O	1:C:239:ALA:N	2.54	0.41
1:C:393:ARG:HG3	1:C:396:PRO:HD3	1.98	0.41
1:D:129:LEU:HD21	1:D:310:GLY:CA	2.50	0.41
1:B:48:ARG:O	1:B:49:LEU:HD23	2.19	0.41
1:B:108:TRP:CH2	1:B:139:LYS:HE2	2.56	0.41
1:B:388:THR:O	1:B:389:VAL:C	2.64	0.41
1:C:35:GLN:O	1:C:39:LEU:HG	2.21	0.41
1:C:142:MET:SD	1:C:144:SER:OG	2.78	0.41
1:C:211:LEU:N	1:C:212:PRO:CD	2.84	0.41
1:D:400:VAL:HG13	1:D:451:GLN:HG2	2.01	0.41
1:A:50:SER:O	1:A:54:ILE:HG13	2.20	0.41
1:A:108:TRP:CZ3	1:A:177:LEU:HB2	2.56	0.41
1:A:289:GLU:OE2	1:A:299:PRO:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:HD21	1:A:472:PRO:HG2	2.01	0.41
1:B:149:GLY:O	1:B:402:HIS:HE1	2.04	0.41
1:B:258:VAL:O	1:B:259:GLY:C	2.64	0.41
1:C:83:MET:HB2	1:C:87:GLU:CD	2.46	0.41
1:C:270:LEU:O	1:C:474:ALA:HB3	2.20	0.41
1:D:54:ILE:HG23	1:D:91:LEU:CD1	2.50	0.41
1:D:312:ALA:O	1:D:316:LEU:HB2	2.20	0.41
1:D:352:VAL:O	1:D:353:ASP:O	2.38	0.41
1:A:331:ALA:HA	1:A:334:LEU:HD12	2.02	0.41
1:A:478:LEU:HB3	1:A:479:PRO:HD2	2.02	0.41
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.81	0.41
1:B:283:HIS:HB2	1:B:417:LEU:HA	2.03	0.41
1:B:293:CYS:O	1:B:334:LEU:HD22	2.21	0.41
1:C:249:ARG:NH1	1:C:249:ARG:HG2	2.35	0.41
1:D:63:ASN:HD22	1:D:63:ASN:H	1.66	0.41
1:D:383:ALA:HA	1:D:384:PRO:HD2	1.95	0.41
1:D:410:ARG:O	1:D:413:GLU:HB3	2.21	0.41
1:A:115:LYS:HG2	1:A:129:LEU:HD12	2.02	0.41
1:A:265:ARG:HD2	1:A:316:LEU:HD13	2.02	0.41
1:A:313:LEU:HD23	1:A:313:LEU:HA	1.84	0.41
1:B:36:LEU:O	1:B:37:PRO:C	2.64	0.41
1:B:211:LEU:N	1:B:212:PRO:HD2	2.36	0.41
1:B:280:CYS:C	1:B:281:VAL:HG23	2.45	0.41
1:B:408:ARG:CG	1:B:413:GLU:HG3	2.31	0.41
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.85	0.41
1:C:191:LEU:O	1:C:192:VAL:HG22	2.19	0.41
1:C:244:ASN:HB3	1:C:247:GLN:CB	2.51	0.41
1:D:331:ALA:O	1:D:334:LEU:HB2	2.21	0.41
1:D:378:GLN:HG2	1:D:441:HIS:ND1	2.36	0.41
1:A:125:VAL:HG23	1:A:277:LEU:CD1	2.51	0.41
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.83	0.41
1:C:401:LEU:N	1:C:401:LEU:HD22	2.36	0.41
1:D:104:TRP:O	1:D:109:ARG:NH1	2.54	0.41
1:D:416:ARG:HB3	1:D:443:ASP:OD1	2.21	0.41
1:A:425:VAL:HG13	1:A:437:TRP:HA	2.03	0.40
1:C:135:ALA:HA	1:C:342:ARG:HH12	1.85	0.40
1:C:145:GLY:O	1:C:155:LEU:HB2	2.21	0.40
1:C:256:VAL:CG2	1:C:266:VAL:HG23	2.51	0.40
1:D:382:LEU:HD22	1:D:434:GLY:O	2.21	0.40
1:D:393:ARG:NH2	1:D:457:GLU:HG2	2.36	0.40
1:A:192:VAL:N	1:A:193:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:LEU:HA	1:B:139:LYS:O	2.20	0.40
1:B:147:GLY:N	1:B:153:GLY:HA3	2.36	0.40
1:C:236:PHE:CD1	1:C:236:PHE:C	2.99	0.40
1:C:329:ARG:HD2	1:C:329:ARG:O	2.21	0.40
1:D:141:PRO:HG2	1:D:225:GLU:OE1	2.21	0.40
1:D:288:GLU:HG2	1:D:372:LEU:CD1	2.51	0.40
1:D:381:LEU:HB3	1:D:437:TRP:HE1	1.86	0.40
1:A:393:ARG:NH2	1:B:178:ASP:OD2	2.54	0.40
1:B:36:LEU:HD23	1:B:39:LEU:HD12	2.04	0.40
1:B:122:GLY:HA2	1:B:286:GLU:OE2	2.21	0.40
1:B:128:VAL:C	1:B:131:PRO:HD2	2.47	0.40
1:B:402:HIS:CG	1:B:407:GLY:HA3	2.57	0.40
1:C:140:VAL:HA	1:C:141:PRO:HD2	2.02	0.40
1:D:155:LEU:HA	1:D:155:LEU:HD23	1.83	0.40
1:A:205:THR:O	1:A:205:THR:CG2	2.69	0.40
1:B:219:LEU:O	1:B:220:SER:C	2.64	0.40
1:C:113:VAL:CB	1:C:313:LEU:HD11	2.48	0.40
1:C:456:GLN:C	1:C:458:ALA:N	2.79	0.40
1:A:285:LEU:CD2	1:A:441:HIS:HD2	2.34	0.40
1:B:63:ASN:HD21	1:B:65:SER:HG	1.57	0.40
1:B:132:ALA:O	1:B:135:ALA:N	2.53	0.40
1:B:313:LEU:HD23	1:B:313:LEU:HA	1.71	0.40
1:B:393:ARG:HB3	1:B:396:PRO:HD2	2.03	0.40
1:C:294:MET:HB3	1:C:340:LEU:CB	2.42	0.40
1:C:356:LEU:O	1:C:360:LEU:HG	2.22	0.40
1:C:364:SER:C	1:C:366:ALA:N	2.79	0.40
1:D:84:ASP:C	1:D:86:GLU:N	2.80	0.40
1:D:192:VAL:N	1:D:193:PRO:HD3	2.36	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	98/482 (20%)	82 (84%)	12 (12%)	4 (4%)	2	13
1	B	72/482 (15%)	62 (86%)	9 (12%)	1 (1%)	9	36
1	C	391/482 (81%)	329 (84%)	45 (12%)	17 (4%)	2	12
1	D	439/482 (91%)	362 (82%)	62 (14%)	15 (3%)	3	17
All	All	1000/1928 (52%)	835 (84%)	128 (13%)	37 (4%)	2	15

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	ASP
1	C	35	GLN
1	C	382	LEU
1	C	425	VAL
1	D	364	SER
1	D	365	PRO
1	D	369	ARG
1	D	414	PRO
1	D	464	ARG
1	A	238	GLY
1	C	238	GLY
1	C	384	PRO
1	D	82	GLY
1	D	106	GLU
1	D	124	LYS
1	B	433	ARG
1	C	34	LYS
1	C	226	GLY
1	C	386	ASP
1	D	203	ASP
1	C	276	PRO
1	C	376	ARG
1	D	98	SER
1	A	257	GLY
1	C	245	GLN
1	C	295	ASP
1	C	354	PRO
1	D	204	VAL
1	D	445	PRO
1	D	462	SER
1	C	243	PRO
1	C	445	PRO
1	A	224	VAL

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Mol	Chain	Res	Type
1	C	82	GLY
1	D	351	GLY
1	D	170	PRO
1	C	414	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	225/359 (63%)	200 (89%)	25 (11%)	6	25
1	B	334/359 (93%)	289 (86%)	45 (14%)	4	18
1	C	332/359 (92%)	307 (92%)	25 (8%)	12	41
1	D	328/359 (91%)	296 (90%)	32 (10%)	7	30
All	All	1219/1436 (85%)	1092 (90%)	127 (10%)	7	28

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	43	LYS
1	A	192	VAL
1	A	203	ASP
1	A	211	LEU
1	A	227	LEU
1	A	273	MET
1	A	277	LEU
1	A	285	LEU
1	A	292	LEU
1	A	295	ASP
1	A	302	LEU
1	A	316	LEU
1	A	319	HIS
1	A	369	ARG
1	A	379	GLU
1	A	381	LEU

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Mol	Chain	Res	Type
1	A	391	LEU
1	A	410	ARG
1	A	431	LEU
1	A	432	ARG
1	A	438	LEU
1	A	459	LEU
1	A	460	VAL
1	A	463	ASP
1	B	38	GLU
1	B	43	LYS
1	B	51	GLU
1	B	63	ASN
1	B	79	ARG
1	B	91	LEU
1	B	100	GLN
1	B	103	GLU
1	B	108	TRP
1	B	124	LYS
1	B	129	LEU
1	B	171	GLU
1	B	174	GLN
1	B	175	VAL
1	B	187	GLN
1	B	211	LEU
1	B	223	LEU
1	B	224	VAL
1	B	230	LEU
1	B	246	GLU
1	B	249	ARG
1	B	256	VAL
1	B	265	ARG
1	B	270	LEU
1	B	277	LEU
1	B	279	ARG
1	B	295	ASP
1	B	302	LEU
1	B	305	LEU
1	B	316	LEU
1	B	340	LEU
1	B	356	LEU
1	B	360	LEU
1	B	374	ARG

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Mol	Chain	Res	Type
1	B	386	ASP
1	B	391	LEU
1	B	400	VAL
1	B	401	LEU
1	B	408	ARG
1	B	409	SER
1	B	410	ARG
1	B	431	LEU
1	B	457	GLU
1	B	459	LEU
1	B	464	ARG
1	C	43	LYS
1	C	49	LEU
1	C	79	ARG
1	C	83	MET
1	C	91	LEU
1	C	97	GLN
1	C	106	GLU
1	C	136	CYS
1	C	154	THR
1	C	214	ILE
1	C	230	LEU
1	C	265	ARG
1	C	273	MET
1	C	305	LEU
1	C	306	VAL
1	C	313	LEU
1	C	369	ARG
1	C	386	ASP
1	C	388	THR
1	C	391	LEU
1	C	397	LEU
1	C	415	LEU
1	C	442	ARG
1	C	463	ASP
1	C	464	ARG
1	D	43	LYS
1	D	51	GLU
1	D	63	ASN
1	D	79	ARG
1	D	101	GLN
1	D	103	GLU

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Mol	Chain	Res	Type
1	D	115	LYS
1	D	140	VAL
1	D	159	GLU
1	D	167	ILE
1	D	205	THR
1	D	223	LEU
1	D	245	GLN
1	D	277	LEU
1	D	305	LEU
1	D	313	LEU
1	D	316	LEU
1	D	340	LEU
1	D	350	GLN
1	D	391	LEU
1	D	401	LEU
1	D	408	ARG
1	D	413	GLU
1	D	415	LEU
1	D	416	ARG
1	D	426	ASP
1	D	456	GLN
1	D	459	LEU
1	D	463	ASP
1	D	464	ARG
1	D	467	PHE
1	D	475	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	245	GLN
1	A	319	HIS
1	A	350	GLN
1	A	429	GLN
1	A	451	GLN
1	A	456	GLN
1	B	63	ASN
1	B	97	GLN
1	B	101	GLN
1	B	187	GLN
1	B	190	GLN

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Mol	Chain	Res	Type
1	B	245	GLN
1	B	319	HIS
1	B	350	GLN
1	B	378	GLN
1	B	456	GLN
1	C	93	GLN
1	C	97	GLN
1	C	101	GLN
1	C	111	GLN
1	C	244	ASN
1	C	247	GLN
1	C	319	HIS
1	C	350	GLN
1	D	35	GLN
1	D	63	ASN
1	D	67	GLN
1	D	93	GLN
1	D	97	GLN
1	D	111	GLN
1	D	244	ASN
1	D	245	GLN
1	D	323	GLN
1	D	325	GLN
1	D	350	GLN
1	D	378	GLN
1	D	451	GLN
1	D	456	GLN

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	1481	-	5,5,5	4.63	5 (100%)	5,5,5	6.20	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1481	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1481	GOL	C3-C2	-7.47	1.23	1.51
2	B	1481	GOL	O1-C1	4.77	1.62	1.42
2	B	1481	GOL	O3-C3	3.90	1.58	1.42
2	B	1481	GOL	C1-C2	-2.74	1.41	1.51
2	B	1481	GOL	O2-C2	-2.38	1.36	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1481	GOL	O3-C3-C2	11.33	161.38	110.38
2	B	1481	GOL	O2-C2-C3	7.15	138.76	109.18
2	B	1481	GOL	O1-C1-C2	3.51	126.19	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1481	GOL	O1-C1-C2-C3
2	B	1481	GOL	C1-C2-C3-O3

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	449/482 (93%)	-0.18	6 (1%) 75 53	15, 19, 40, 57	0
1	B	448/482 (92%)	-0.11	6 (1%) 75 53	15, 18, 40, 66	0
1	C	445/482 (92%)	0.20	6 (1%) 75 53	15, 33, 56, 68	0
1	D	445/482 (92%)	0.20	13 (2%) 53 31	15, 33, 58, 68	0
All	All	1787/1928 (92%)	0.03	31 (1%) 69 45	15, 25, 53, 68	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	363	GLY	7.8
1	D	480	PRO	4.3
1	C	83	MET	3.5
1	D	364	SER	3.2
1	A	297	ALA	3.0
1	B	283	HIS	3.0
1	D	466	PRO	2.8
1	A	480	PRO	2.8
1	C	269	ALA	2.6
1	D	415	LEU	2.6
1	B	108	TRP	2.5
1	D	361	CYS	2.4
1	D	470	PRO	2.4
1	B	409	SER	2.4
1	D	465	ALA	2.4
1	C	82	GLY	2.4
1	C	448	SER	2.3
1	A	32	GLU	2.3
1	B	480	PRO	2.3
1	D	468	ALA	2.2
1	B	109	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	2.1
1	A	248	ALA	2.1
1	A	412	GLY	2.1
1	D	241	VAL	2.0
1	D	436	PRO	2.0
1	B	481	GLN	2.0
1	D	101	GLN	2.0
1	D	414	PRO	2.0
1	C	421	ALA	2.0
1	C	469	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($\text{\AA}^2$)	Q<0.9
2	GOL	B	1481	6/6	0.85	0.14	24,28,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.