Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 09:14 PM EDT

PDB ID	:	2ZOQ
Title	:	Structural dissection of human mitogen-activated kinase ERK1
Authors	:	Kinoshita, T.; Tada, T.; Nakae, S.; Yoshida, I.
Deposited on	:	2008-06-01
Resolution	:	2.39 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

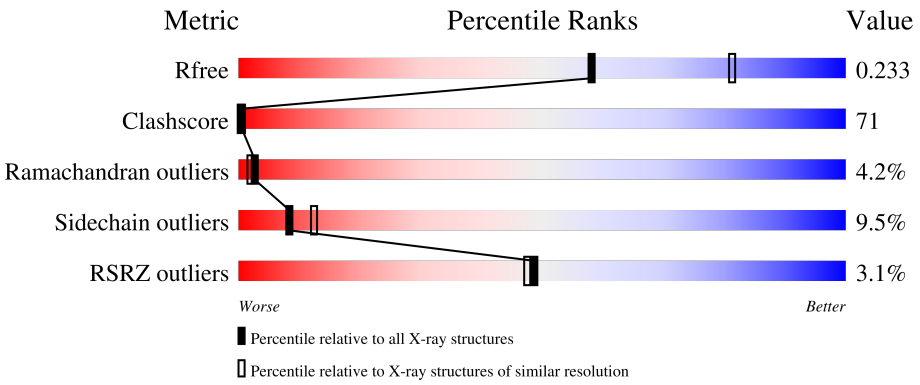
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	382	3% 29% 51% 10% • 8%
1	B	382	3% 35% 47% 9% • 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
1	PTR	B	204	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6102 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.

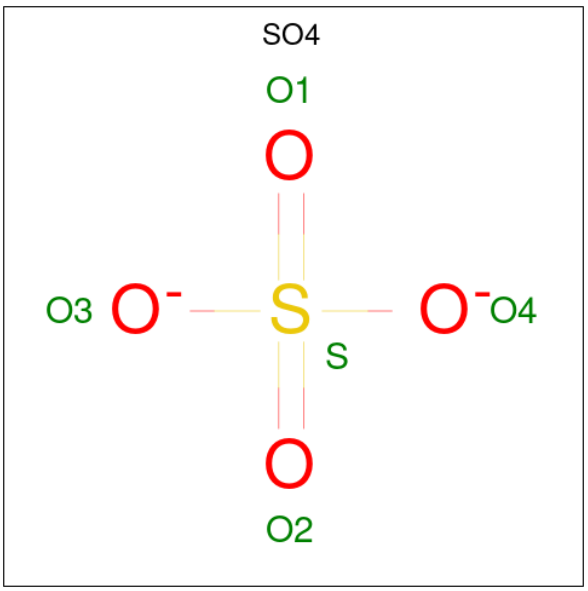
- Molecule 1 is a protein called Mitogen-activated protein kinase 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	352	2868	1834	490	528	1	15	0	0	0
1	B	352	2868	1834	490	528	1	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	LEU	-	expression tag	UNP P27361
A	-1	GLY	-	expression tag	UNP P27361
A	0	SER	-	expression tag	UNP P27361
B	-2	LEU	-	expression tag	UNP P27361
B	-1	GLY	-	expression tag	UNP P27361
B	0	SER	-	expression tag	UNP P27361

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

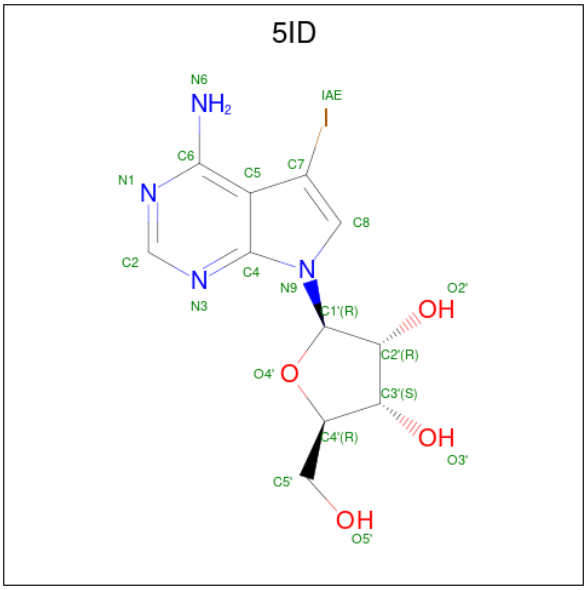


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	1	1	1	0	0
			Total	Na		
3	B	1	1	1	0	0

- Molecule 4 is (2R,3R,4S,5R)-2-(4-AMINO-5-IODO-7H-PYRROLO[2,3-D]PYRIMIDIN-7-YL)-5-(HYDROXYMETHYL)TETRAHYDROFURAN-3,4-DIOL (three-letter code: 5ID) (formula: $C_{11}H_{13}IN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	I	N	O		
4	A	1	20	11	1	4	4	0	0
			Total	C	I	N	O		
4	B	1	20	11	1	4	4	0	0

- Molecule 5 is water.

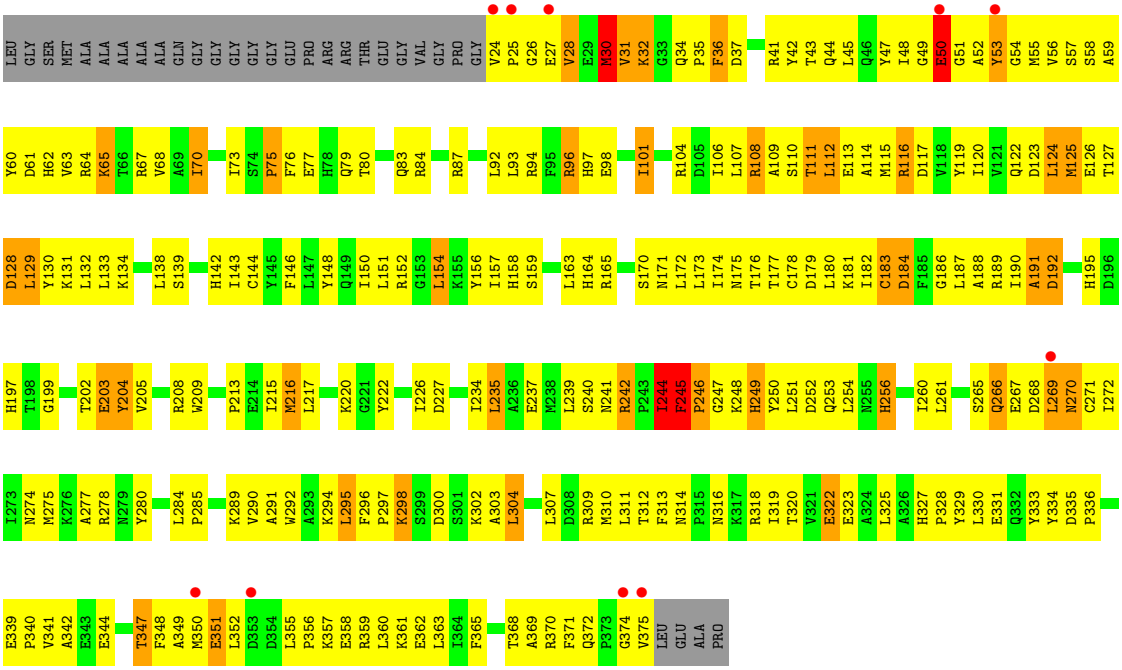
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	158	158	158	0	0
			Total	O		
5	B	156	156	156	0	0

3 Residue-property plots (i)

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

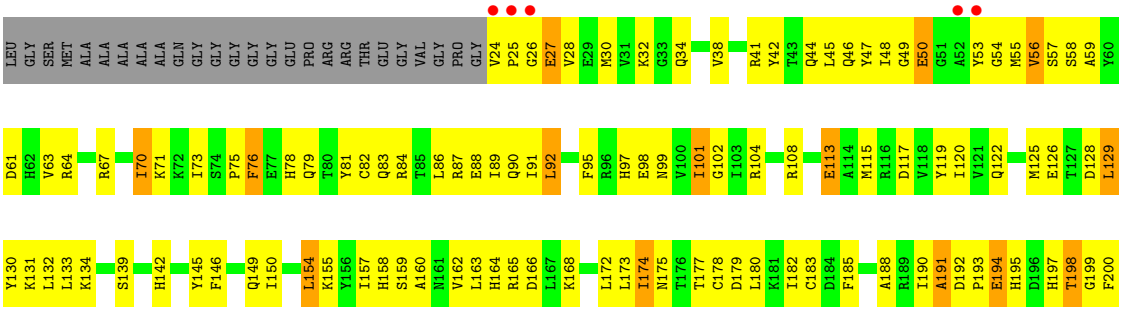
• Molecule 1: Mitogen-activated protein kinase 3

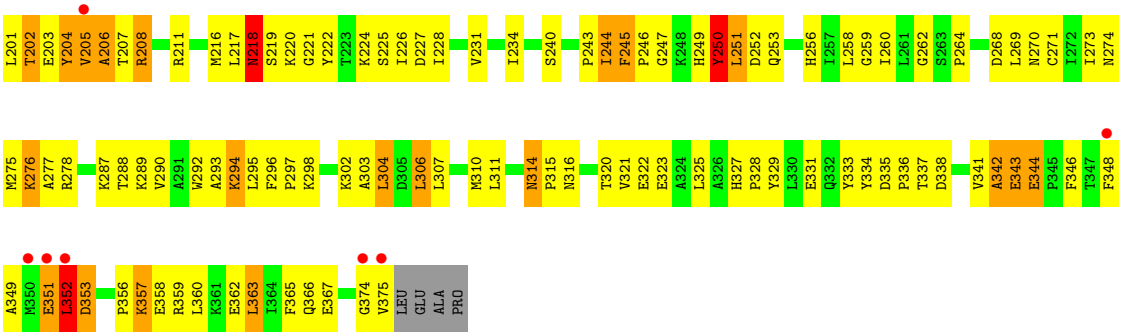
Chain A: 3% 29% 51% 10% • 8%



• Molecule 1: Mitogen-activated protein kinase 3

Chain B: 3% 35% 47% 9% • 8%




L201 T202 E203 Y204 V205 A206 T207 R208 R211 M216 L217 N218 S219 K220 G221 Y222 T223 K224 S225 I226 D227 I228 V231 I234 S240 P243 I244 F245 P246 G247 K248 H249 Y250 L251 D252 Q253 H256 I257 L258 G259 I260 L261 G262 S263 P264 D268 L269 N270 C271 I272 I273 N274
M275 K276 A277 R278 K287 T288 K289 V290 A291 W292 A293 K294 L295 F296 P297 K298 K302 A303 L304 D305 L306 L307 M310 L311 N314 P315 N316 T320 V321 E322 E323 A324 L325 A326 H327 P328 Y329 L330 E331 Q332 Y333 Y334 D335 P336 T337 D338 V341 A342 E343 E344 P345 F346 T347 F348
A349 M350 E351 L352 D353 P356 K357 E358 R359 L360 K361 E362 L363 I364 F365 Q366 E367 G374 V375 LEU GLU ALA PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.38Å 91.54Å 64.93Å 90.00° 91.50° 90.00°	Depositor
Resolution (Å)	45.57 – 2.39 45.57 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.57-2.39) 99.4 (45.57-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.53 (at 2.39Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.249 , 0.267 0.240 , 0.233	Depositor DCC
R_{free} test set	1457 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.004 for l,k,-h 0.148 for h,-k,-l 0.019 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6102	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 5ID, PTR, NA

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	0.35	0/2916	0.72	8/3948 (0.2%)
1	B	0.37	2/2916 (0.1%)	0.71	7/3948 (0.2%)
All	All	0.36	2/5832 (0.0%)	0.72	15/7896 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	GLU	CD-OE2	-5.89	1.19	1.25
1	B	251	LEU	C-N	5.08	1.45	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	TYR	O-C-N	-10.50	105.89	122.70
1	A	244	ILE	N-CA-C	9.16	135.74	111.00
1	B	351	GLU	CA-CB-CG	-8.21	95.34	113.40
1	A	244	ILE	C-N-CA	7.66	140.84	121.70
1	B	174	ILE	CA-CB-CG1	-7.26	97.20	111.00
1	A	50	GLU	CA-CB-CG	-6.38	99.38	113.40
1	A	50	GLU	CG-CD-OE1	6.31	130.92	118.30
1	A	244	ILE	CA-C-N	6.24	130.92	117.20
1	A	50	GLU	CG-CD-OE2	-6.17	105.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	245	PHE	N-CA-C	6.01	127.23	111.00
1	A	31	VAL	N-CA-C	-5.86	95.17	111.00
1	B	50	GLU	CB-CG-CD	-5.70	98.83	114.20
1	B	50	GLU	CA-CB-CG	5.54	125.58	113.40
1	B	244	ILE	N-CA-C	-5.18	97.00	111.00
1	B	352	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	TYR	Mainchain

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	2868	0	2871	463	0
1	B	2868	0	2871	379	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	20	0	13	2	0
4	B	20	0	13	3	0
5	A	158	0	0	19	0
5	B	156	0	0	24	0
All	All	6102	0	5768	822	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 71.

All (822) 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:248:LYS:CB	1:A:249:HIS:HB2	1.51	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LYS:HB2	1:A:249:HIS:CB	1.61	1.28
1:A:53:TYR:CE1	1:A:186:GLY:HA3	1.68	1.27
1:A:270:ASN:N	1:A:271:CYS:HB2	1.51	1.26
1:A:265:SER:OG	1:A:268:ASP:HB2	1.39	1.18
1:B:352:LEU:HD23	5:B:492:HOH:O	1.44	1.17
1:A:319:ILE:HG12	1:A:323:GLU:HG3	1.27	1.14
1:A:269:LEU:HB2	1:A:270:ASN:CB	1.77	1.14
1:A:269:LEU:HB2	1:A:270:ASN:HB2	1.27	1.12
1:A:270:ASN:H	1:A:271:CYS:CB	1.61	1.11
1:A:344:GLU:HG3	1:B:276:LYS:HE3	1.29	1.11
1:A:27:GLU:OE2	1:A:37:ASP:HA	1.48	1.10
1:A:50:GLU:HG2	1:A:51:GLY:H	0.95	1.10
1:B:357:LYS:H	1:B:357:LYS:HD3	1.00	1.09
1:A:245:PHE:HB2	5:A:384:HOH:O	1.52	1.09
1:A:349:ALA:HA	1:A:350:MET:CB	1.83	1.08
1:A:349:ALA:CA	1:A:350:MET:HB2	1.84	1.08
1:B:203:GLU:HB2	1:B:204:PTR:CB	1.85	1.07
1:A:50:GLU:CG	1:A:51:GLY:H	1.64	1.06
1:A:111:THR:HG23	1:A:114:ALA:HB3	1.39	1.04
1:B:101:ILE:HD11	1:B:183:CYS:HA	1.36	1.02
1:A:112:LEU:CD2	1:A:361:LYS:HE3	1.89	1.02
1:B:203:GLU:CB	1:B:204:PTR:HB3	1.89	1.02
1:B:79:GLN:HB2	1:B:357:LYS:HD2	1.40	1.02
1:A:116:ARG:HH21	1:A:116:ARG:HG3	1.20	1.01
1:A:159:SER:CB	1:A:341:VAL:HG22	1.91	1.00
1:B:83:GLN:OE1	1:B:353:ASP:HA	1.61	1.00
1:A:112:LEU:HD21	1:A:361:LYS:HE3	1.44	0.99
1:A:270:ASN:H	1:A:271:CYS:CA	1.73	0.99
1:B:357:LYS:H	1:B:357:LYS:CD	1.72	0.99
1:B:259:GLY:HA2	1:B:287:LYS:HE2	1.46	0.98
1:A:269:LEU:CB	1:A:270:ASN:HB2	1.93	0.97
1:B:78:HIS:HB2	1:B:81:TYR:HD2	1.27	0.97
1:B:357:LYS:HD3	1:B:357:LYS:N	1.76	0.97
1:B:64:ARG:NH2	1:B:104:ARG:HH11	1.62	0.96
1:A:269:LEU:C	1:A:272:ILE:HG12	1.85	0.96
1:B:207:THR:O	1:B:208:ARG:HB2	1.62	0.96
1:A:50:GLU:HG2	1:A:51:GLY:N	1.80	0.96
1:A:319:ILE:CG1	1:A:323:GLU:HG3	1.93	0.96
1:A:242:ARG:HB2	1:A:242:ARG:HH21	1.29	0.96
1:B:205:VAL:HG12	1:B:206:ALA:H	1.30	0.95
1:B:203:GLU:HB2	1:B:204:PTR:HB3	0.97	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASN:ND2	1:A:179:ASP:HB2	1.81	0.95
1:B:157:ILE:HD11	1:B:162:VAL:CG1	1.96	0.95
1:A:328:PRO:HA	1:A:331:GLU:HG2	1.48	0.94
1:B:64:ARG:HH21	1:B:104:ARG:HH11	1.11	0.94
1:B:298:LYS:O	1:B:298:LYS:HD3	1.68	0.94
1:B:357:LYS:HA	1:B:360:LEU:HD23	1.48	0.94
1:A:53:TYR:HE1	1:A:186:GLY:HA3	1.06	0.93
1:B:175:ASN:ND2	1:B:179:ASP:HB2	1.84	0.93
1:A:349:ALA:HA	1:A:350:MET:HB2	0.94	0.93
1:B:64:ARG:HD3	1:B:104:ARG:NH1	1.83	0.92
1:A:126:GLU:HG2	1:A:175:ASN:HA	1.50	0.92
1:A:270:ASN:H	1:A:271:CYS:HB2	1.13	0.92
1:A:375:VAL:HA	1:B:320:THR:HG21	1.52	0.92
1:A:27:GLU:HG3	1:A:28:VAL:HG13	1.50	0.91
1:A:270:ASN:N	1:A:271:CYS:CB	2.29	0.90
1:B:198:THR:OG1	1:B:202:THR:HG21	1.71	0.90
1:A:41:ARG:CD	1:A:63:VAL:HG13	2.01	0.90
1:B:276:LYS:NZ	1:B:276:LYS:H	1.70	0.90
1:A:116:ARG:HG3	1:A:116:ARG:NH2	1.84	0.89
1:A:298:LYS:HB2	1:A:298:LYS:NZ	1.88	0.89
1:B:228:ILE:HD12	1:B:228:ILE:H	1.37	0.89
1:B:159:SER:HB2	1:B:341:VAL:HG13	1.54	0.89
1:B:90:GLN:NE2	1:B:348:PHE:HE1	1.70	0.88
1:A:27:GLU:O	1:A:28:VAL:HG22	1.73	0.88
1:A:235:LEU:HD12	1:A:310:MET:CE	2.05	0.87
1:B:79:GLN:CB	1:B:357:LYS:HD2	2.03	0.87
1:A:126:GLU:HG3	1:A:176:THR:HG23	1.57	0.87
1:A:159:SER:HB2	1:A:341:VAL:HG22	1.53	0.87
1:B:221:GLY:HA2	1:B:226:ILE:HG13	1.56	0.86
1:A:344:GLU:CD	1:B:276:LYS:HE2	1.96	0.86
1:A:355:LEU:HD21	1:A:359:ARG:HB2	1.55	0.86
1:A:52:ALA:HB2	5:A:541:HOH:O	1.75	0.86
1:A:27:GLU:CD	1:A:28:VAL:H	1.78	0.86
1:A:101:ILE:HD12	1:A:182:ILE:O	1.76	0.86
1:A:48:ILE:HD11	1:A:58:SER:HB3	1.58	0.85
1:B:328:PRO:HA	1:B:331:GLU:HG2	1.59	0.85
1:B:302:LYS:HE2	1:B:328:PRO:HB2	1.58	0.85
1:B:95:PHE:HE2	1:B:157:ILE:HD13	1.42	0.84
1:B:203:GLU:HB3	1:B:204:PTR:CD1	2.07	0.84
1:B:203:GLU:HB3	1:B:204:PTR:HD1	1.57	0.84
1:A:359:ARG:HD3	1:A:362:GLU:OE1	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ARG:HB2	1:A:242:ARG:NH2	1.93	0.83
1:B:275:MET:HB3	1:B:276:LYS:NZ	1.92	0.83
1:B:205:VAL:HG12	1:B:206:ALA:N	1.93	0.83
1:B:245:PHE:N	1:B:246:PRO:HD3	1.91	0.83
1:B:46:GLN:HB2	1:B:58:SER:OG	1.80	0.82
1:A:249:HIS:CG	1:A:252:ASP:HB2	2.14	0.82
1:A:128:ASP:OD2	1:A:170:SER:HA	1.79	0.82
1:B:90:GLN:HE21	1:B:348:PHE:HE1	1.25	0.82
1:B:228:ILE:HD12	1:B:228:ILE:N	1.95	0.82
1:A:269:LEU:CA	1:A:270:ASN:HB2	2.09	0.81
1:A:269:LEU:O	1:A:272:ILE:HG12	1.80	0.81
1:B:159:SER:CB	1:B:341:VAL:HG13	2.10	0.81
1:B:157:ILE:CD1	1:B:162:VAL:HB	2.08	0.81
1:A:30:MET:HE2	1:A:35:PRO:HA	1.60	0.81
1:A:36:PHE:HB3	1:A:45:LEU:CD2	2.10	0.81
1:B:208:ARG:NH2	1:B:249:HIS:HA	1.95	0.81
1:A:266:GLN:O	1:A:269:LEU:HD13	1.81	0.80
1:B:199:GLY:O	1:B:202:THR:CG2	2.28	0.80
1:B:276:LYS:H	1:B:276:LYS:HZ1	1.28	0.80
1:A:269:LEU:N	1:A:270:ASN:HB2	1.96	0.80
1:A:344:GLU:HG3	1:B:276:LYS:CE	2.08	0.80
1:B:256:HIS:O	1:B:260:ILE:HD13	1.81	0.80
1:B:59:ALA:N	1:B:67:ARG:HH22	1.79	0.80
1:A:43:THR:OG1	1:A:62:HIS:HE1	1.65	0.80
1:B:294:LYS:HA	1:B:294:LYS:HE3	1.64	0.79
1:A:349:ALA:CB	1:A:352:LEU:H	1.95	0.79
1:A:64:ARG:HH22	1:A:104:ARG:HG3	1.44	0.79
1:A:349:ALA:HB2	1:A:352:LEU:HG	1.62	0.79
1:A:54:GLY:HA2	5:A:488:HOH:O	1.83	0.79
1:B:306:LEU:HD22	1:B:310:MET:CE	2.12	0.79
1:A:73:ILE:HG22	1:A:75:PRO:HD3	1.65	0.78
1:A:344:GLU:CG	1:B:276:LYS:HE3	2.12	0.78
1:A:128:ASP:OD1	1:A:131:LYS:HG3	1.84	0.78
1:B:173:LEU:HD11	1:B:183:CYS:SG	2.23	0.78
1:A:116:ARG:HH21	1:A:116:ARG:CG	1.97	0.77
1:A:270:ASN:H	1:A:271:CYS:C	1.88	0.77
1:B:252:ASP:OD1	1:B:256:HIS:HD2	1.67	0.77
1:A:267:GLU:O	1:A:270:ASN:HB3	1.85	0.77
1:A:244:ILE:HG13	1:A:244:ILE:O	1.83	0.77
1:A:112:LEU:HD22	1:A:361:LYS:HE3	1.65	0.76
1:B:78:HIS:CB	1:B:81:TYR:HD2	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:GLU:OE1	1:A:361:LYS:HE2	1.85	0.76
1:A:175:ASN:HD21	1:A:179:ASP:HB2	1.50	0.76
1:B:276:LYS:NZ	1:B:276:LYS:N	2.33	0.76
1:A:31:VAL:O	1:A:32:LYS:HB2	1.86	0.76
1:B:275:MET:HB3	1:B:276:LYS:HZ1	1.49	0.76
1:A:250:TYR:O	1:A:251:LEU:HB3	1.85	0.76
1:A:53:TYR:CE1	1:A:186:GLY:CA	2.62	0.75
1:A:50:GLU:CG	1:A:51:GLY:N	2.33	0.75
1:B:70:ILE:HD11	1:B:119:TYR:HB3	1.69	0.75
1:A:269:LEU:HD22	1:A:270:ASN:ND2	2.02	0.75
1:B:129:LEU:CD1	1:B:133:LEU:HG	2.16	0.75
1:B:306:LEU:HD22	1:B:310:MET:HE1	1.68	0.75
1:B:314:ASN:ND2	1:B:316:ASN:H	1.85	0.75
1:B:247:GLY:HA2	1:B:252:ASP:OD1	1.87	0.75
1:A:269:LEU:HD22	1:A:270:ASN:HD22	1.52	0.75
1:B:357:LYS:CA	1:B:360:LEU:HD23	2.16	0.74
1:B:314:ASN:C	1:B:314:ASN:HD22	1.91	0.74
1:A:269:LEU:CB	1:A:270:ASN:CB	2.57	0.74
1:A:350:MET:O	1:A:351:GLU:HB3	1.87	0.74
1:A:132:LEU:HD23	1:A:132:LEU:O	1.87	0.74
1:A:205:VAL:HB	5:A:483:HOH:O	1.88	0.74
1:A:143:ILE:HD13	1:A:239:LEU:HD23	1.70	0.74
1:A:191:ALA:O	1:A:192:ASP:HB3	1.86	0.73
1:B:139:SER:HG	1:B:142:HIS:CG	2.06	0.73
1:A:49:GLY:O	1:A:50:GLU:O	2.06	0.73
1:A:320:THR:OG1	1:A:323:GLU:HG2	1.88	0.73
1:B:129:LEU:HD12	1:B:133:LEU:HG	1.70	0.73
1:B:28:VAL:HA	5:B:452:HOH:O	1.88	0.73
1:A:355:LEU:HD22	1:A:360:LEU:HG	1.71	0.73
1:A:120:ILE:HD12	1:A:120:ILE:N	2.04	0.73
1:B:70:ILE:HD12	1:B:71:LYS:N	2.03	0.73
1:A:289:LYS:HD2	5:A:456:HOH:O	1.88	0.73
1:B:203:GLU:CB	1:B:204:PTR:HD1	2.18	0.73
1:B:64:ARG:HH21	1:B:104:ARG:NH1	1.84	0.73
1:B:328:PRO:HA	1:B:331:GLU:CG	2.19	0.73
1:A:133:LEU:HD13	1:A:237:GLU:HG2	1.71	0.72
1:A:269:LEU:HB2	1:A:270:ASN:HD22	1.54	0.72
1:A:350:MET:O	1:A:351:GLU:CB	2.37	0.72
1:A:248:LYS:CA	1:A:249:HIS:HB2	2.20	0.72
1:B:343:GLU:HG3	1:B:344:GLU:N	2.04	0.72
1:A:64:ARG:O	1:A:65:LYS:HD2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASP:OD2	1:A:195:HIS:HD2	1.72	0.72
1:A:244:ILE:HG12	1:A:245:PHE:CE1	2.25	0.72
1:A:41:ARG:HD3	1:A:63:VAL:HG13	1.70	0.72
1:A:41:ARG:HD3	1:A:63:VAL:CG1	2.19	0.72
1:B:49:GLY:HA3	5:B:514:HOH:O	1.89	0.72
1:A:349:ALA:HB3	1:A:352:LEU:HB2	1.72	0.71
1:A:246:PRO:O	1:A:253:GLN:OE1	2.08	0.71
1:A:269:LEU:HB2	1:A:270:ASN:ND2	2.04	0.71
1:A:291:ALA:O	1:A:295:LEU:HD12	1.90	0.71
1:B:352:LEU:CD2	5:B:492:HOH:O	2.15	0.71
1:B:207:THR:O	1:B:208:ARG:CB	2.39	0.71
1:A:94:ARG:HG2	1:B:197:HIS:CD2	2.26	0.71
1:B:64:ARG:NH2	1:B:104:ARG:NH1	2.37	0.71
1:A:30:MET:CE	1:A:35:PRO:HA	2.21	0.70
1:B:335:ASP:OD1	1:B:337:THR:HB	1.91	0.70
1:A:297:PRO:O	1:A:298:LYS:HB3	1.90	0.70
1:A:269:LEU:C	1:A:271:CYS:HB2	2.11	0.70
1:A:165:ARG:CZ	1:A:189:ARG:HD3	2.21	0.70
1:A:270:ASN:CA	1:A:272:ILE:H	2.05	0.70
1:A:298:LYS:HB2	1:A:298:LYS:HZ2	1.56	0.70
1:A:111:THR:CG2	1:A:114:ALA:HB3	2.17	0.70
1:A:349:ALA:HB1	1:A:352:LEU:H	1.56	0.70
1:A:163:LEU:HD11	1:A:191:ALA:HA	1.73	0.69
1:A:269:LEU:HD23	1:A:278:ARG:NH2	2.06	0.69
1:A:344:GLU:CG	1:B:276:LYS:CE	2.69	0.69
1:A:28:VAL:HG23	1:A:28:VAL:O	1.92	0.69
1:B:205:VAL:CG1	1:B:206:ALA:H	1.97	0.69
1:B:175:ASN:HD21	1:B:179:ASP:HB2	1.58	0.69
1:B:95:PHE:CE2	1:B:157:ILE:HD13	2.26	0.69
1:B:198:THR:CG2	1:B:220:LYS:HG2	2.22	0.69
1:A:108:ARG:HG3	1:A:115:MET:SD	2.33	0.68
1:A:240:SER:OG	1:A:296:PHE:HE1	1.75	0.68
1:B:228:ILE:H	1:B:228:ILE:CD1	2.04	0.68
1:B:342:ALA:O	1:B:343:GLU:HG2	1.92	0.68
1:A:41:ARG:NE	1:A:63:VAL:HG22	2.09	0.68
1:B:260:ILE:HD12	1:B:260:ILE:N	2.09	0.68
1:A:195:HIS:O	1:A:220:LYS:HD2	1.94	0.68
1:A:319:ILE:HG12	1:A:323:GLU:CG	2.17	0.68
1:B:34:GLN:HG3	1:B:55:MET:CE	2.23	0.68
1:A:349:ALA:CB	1:A:352:LEU:HG	2.24	0.68
1:B:154:LEU:HA	1:B:157:ILE:CG2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:SER:HB3	1:A:341:VAL:CG2	2.22	0.68
1:A:320:THR:HG23	1:A:323:GLU:OE2	1.95	0.67
1:B:78:HIS:HB2	1:B:81:TYR:CD2	2.19	0.67
1:A:244:ILE:HG23	1:A:245:PHE:CD2	2.30	0.67
1:B:190:ILE:HG12	1:B:348:PHE:CD2	2.29	0.67
1:A:269:LEU:CB	1:A:270:ASN:CA	2.73	0.67
1:A:350:MET:SD	1:B:278:ARG:NH2	2.67	0.67
1:A:355:LEU:HG	1:A:356:PRO:HD2	1.76	0.67
1:A:128:ASP:OD2	1:A:130:TYR:HB3	1.95	0.67
1:B:46:GLN:O	1:B:57:SER:HB2	1.95	0.67
1:A:41:ARG:CZ	1:A:63:VAL:HG22	2.25	0.66
1:B:90:GLN:NE2	1:B:348:PHE:CE1	2.61	0.66
1:A:270:ASN:N	1:A:272:ILE:N	2.42	0.66
1:B:157:ILE:HD11	1:B:162:VAL:CB	2.25	0.66
1:B:157:ILE:HD12	1:B:162:VAL:HB	1.75	0.66
1:A:240:SER:OG	1:A:296:PHE:CE1	2.47	0.66
1:A:154:LEU:HD23	1:A:157:ILE:CG2	2.26	0.66
1:B:70:ILE:CD1	1:B:119:TYR:HB3	2.25	0.66
1:B:224:LYS:O	1:B:228:ILE:CD1	2.43	0.66
1:B:211:ARG:HG2	5:B:504:HOH:O	1.95	0.66
1:A:36:PHE:HB3	1:A:45:LEU:HD21	1.77	0.66
1:A:65:LYS:HD2	1:A:65:LYS:O	1.95	0.66
1:B:218:ASN:C	1:B:218:ASN:HD22	1.97	0.66
1:B:259:GLY:HA2	1:B:287:LYS:CE	2.24	0.66
1:B:27:GLU:HG3	1:B:28:VAL:H	1.61	0.66
1:A:159:SER:CB	1:A:341:VAL:CG2	2.71	0.66
1:A:189:ARG:NE	1:A:222:TYR:CE1	2.64	0.66
1:A:265:SER:O	1:A:268:ASP:HB3	1.96	0.65
1:B:173:LEU:CD1	1:B:183:CYS:SG	2.85	0.65
1:A:108:ARG:HH22	1:A:369:ALA:HA	1.61	0.65
1:B:194:GLU:H	1:B:194:GLU:CD	1.99	0.65
1:B:227:ASP:O	1:B:231:VAL:HG23	1.97	0.65
1:A:41:ARG:HH11	1:A:61:ASP:CG	2.00	0.65
1:B:41:ARG:HH11	1:B:63:VAL:HG22	1.61	0.65
1:A:24:VAL:HG12	1:A:24:VAL:O	1.95	0.65
1:A:43:THR:OG1	1:A:62:HIS:CE1	2.49	0.65
1:A:65:LYS:O	1:A:65:LYS:CD	2.45	0.65
1:B:157:ILE:HD11	1:B:162:VAL:HG11	1.78	0.65
1:A:65:LYS:HD2	1:A:65:LYS:C	2.17	0.64
1:A:268:ASP:OD2	1:A:313:PHE:HD2	1.81	0.64
1:A:280:TYR:CE2	1:A:284:LEU:HD11	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HD12	1:B:45:LEU:N	2.12	0.64
1:B:202:THR:OG1	5:B:569:HOH:O	2.15	0.64
1:B:294:LYS:HE3	1:B:294:LYS:CA	2.27	0.64
1:A:113:GLU:CD	1:A:113:GLU:H	2.01	0.64
1:A:235:LEU:HD12	1:A:310:MET:HE3	1.79	0.64
1:A:27:GLU:O	1:A:28:VAL:CG2	2.44	0.64
1:A:31:VAL:O	1:A:31:VAL:HG23	1.96	0.64
1:A:199:GLY:HA2	1:A:274:ASN:HD21	1.63	0.64
1:A:246:PRO:HD2	1:A:256:HIS:CD2	2.32	0.64
1:A:285:PRO:HA	5:A:435:HOH:O	1.97	0.64
1:A:298:LYS:HB2	1:A:298:LYS:HZ3	1.62	0.64
1:B:165:ARG:NH2	1:B:221:GLY:O	2.31	0.64
1:B:293:ALA:HB3	1:B:294:LYS:NZ	2.12	0.64
1:B:27:GLU:HG3	1:B:28:VAL:N	2.13	0.64
1:A:31:VAL:HG23	1:A:55:MET:SD	2.37	0.64
1:B:41:ARG:NH1	1:B:63:VAL:CG2	2.61	0.64
1:B:293:ALA:HB3	1:B:294:LYS:HZ2	1.62	0.64
1:B:342:ALA:O	1:B:343:GLU:CB	2.46	0.64
1:B:348:PHE:HB3	1:B:352:LEU:HD22	1.80	0.63
1:A:27:GLU:OE2	1:A:28:VAL:N	2.30	0.63
1:A:249:HIS:ND1	1:A:252:ASP:HB2	2.13	0.63
1:B:125:MET:HG3	1:B:173:LEU:HB3	1.81	0.63
1:B:190:ILE:HG12	1:B:348:PHE:HD2	1.62	0.63
1:A:41:ARG:CZ	1:A:63:VAL:CG2	2.76	0.63
1:A:36:PHE:CD2	1:A:45:LEU:HD23	2.33	0.63
1:B:154:LEU:HA	1:B:157:ILE:HG22	1.79	0.63
1:A:355:LEU:HD21	1:A:359:ARG:CB	2.28	0.63
1:B:206:ALA:HB3	5:B:504:HOH:O	1.98	0.63
1:A:122:GLN:OE1	4:A:382:5ID:IAE	2.87	0.62
1:B:314:ASN:HD22	1:B:316:ASN:H	1.45	0.62
1:A:133:LEU:CD1	1:A:237:GLU:HG2	2.29	0.62
1:B:157:ILE:HD11	1:B:162:VAL:HB	1.78	0.62
1:B:203:GLU:CB	1:B:204:PTR:CD1	2.76	0.62
1:B:203:GLU:CB	1:B:204:PTR:CB	2.64	0.62
1:A:31:VAL:HG21	1:A:36:PHE:CE1	2.34	0.62
1:A:344:GLU:OE2	1:B:276:LYS:HE2	1.98	0.62
1:B:78:HIS:CB	1:B:81:TYR:CD2	2.81	0.62
1:B:276:LYS:HZ1	1:B:276:LYS:N	1.93	0.62
1:B:128:ASP:OD1	1:B:131:LYS:HG2	2.00	0.62
1:B:24:VAL:HB	1:B:25:PRO:CD	2.29	0.62
1:B:199:GLY:O	1:B:202:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:N	1:A:67:ARG:HH22	1.97	0.62
1:A:208:ARG:NH2	1:A:247:GLY:O	2.32	0.62
1:A:36:PHE:CB	1:A:45:LEU:CD2	2.77	0.62
1:A:53:TYR:OH	1:A:187:LEU:HD22	2.00	0.61
1:A:240:SER:HG	1:A:296:PHE:HE1	1.44	0.61
1:A:268:ASP:OD2	1:A:313:PHE:CD2	2.54	0.61
1:B:76:PHE:HA	1:B:82:CYS:SG	2.40	0.61
1:A:27:GLU:CD	1:A:37:ASP:HA	2.21	0.61
1:A:126:GLU:HG3	1:A:176:THR:H	1.66	0.61
1:A:190:ILE:O	1:A:191:ALA:O	2.17	0.61
1:A:269:LEU:HB2	1:A:270:ASN:CA	2.29	0.61
1:A:303:ALA:HB2	1:A:329:TYR:CZ	2.36	0.61
1:B:101:ILE:HG12	1:B:183:CYS:HB3	1.82	0.61
1:B:307:LEU:CD1	1:B:311:LEU:HD12	2.31	0.61
1:A:191:ALA:O	1:A:192:ASP:CB	2.47	0.61
1:A:83:GLN:O	1:A:87:ARG:HG3	2.00	0.61
1:A:199:GLY:O	1:A:202:THR:HG23	2.01	0.61
1:B:24:VAL:HB	1:B:25:PRO:HD3	1.81	0.61
1:A:144:CYS:HG	1:A:333:TYR:HE2	1.48	0.61
1:A:355:LEU:C	1:A:355:LEU:HD23	2.20	0.61
1:B:298:LYS:HD3	1:B:298:LYS:C	2.20	0.61
1:A:31:VAL:CG2	1:A:36:PHE:CE1	2.84	0.61
1:A:104:ARG:NH2	1:A:123:ASP:OD2	2.33	0.61
1:A:125:MET:HE1	1:A:181:LYS:HE3	1.83	0.61
1:A:269:LEU:HB2	1:A:270:ASN:CG	2.21	0.61
1:A:303:ALA:HB2	1:A:329:TYR:CE1	2.35	0.61
1:A:53:TYR:HE1	1:A:186:GLY:CA	1.96	0.60
1:A:112:LEU:HD22	1:A:361:LYS:CE	2.30	0.60
1:A:172:LEU:HD11	1:A:234:ILE:HD13	1.82	0.60
1:A:245:PHE:CE1	1:A:260:ILE:HD12	2.36	0.60
1:A:268:ASP:O	1:A:269:LEU:O	2.19	0.60
1:A:344:GLU:CD	1:B:276:LYS:CE	2.68	0.60
1:B:193:PRO:HD2	1:B:194:GLU:OE1	2.01	0.60
1:A:70:ILE:HD11	1:A:119:TYR:HB3	1.82	0.60
1:A:126:GLU:HG2	1:A:175:ASN:CA	2.27	0.60
1:A:248:LYS:CA	1:A:249:HIS:CB	2.78	0.60
1:B:252:ASP:OD1	1:B:256:HIS:CD2	2.52	0.60
1:B:298:LYS:O	1:B:298:LYS:CD	2.48	0.60
1:A:267:GLU:OE2	1:A:267:GLU:N	2.35	0.60
1:B:307:LEU:HD11	1:B:311:LEU:HD12	1.83	0.60
1:B:44:GLN:HG3	1:B:44:GLN:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:N	1:A:271:CYS:C	2.55	0.60
1:A:350:MET:SD	1:B:278:ARG:CZ	2.90	0.60
1:B:64:ARG:HD3	1:B:104:ARG:CZ	2.32	0.60
1:B:157:ILE:HD11	1:B:162:VAL:HG12	1.82	0.60
1:B:203:GLU:HA	1:B:204:PTR:HD1	1.84	0.60
1:A:126:GLU:HG3	1:A:176:THR:CG2	2.30	0.59
1:B:200:PHE:CE1	1:B:277:ALA:HA	2.37	0.59
1:A:235:LEU:HD12	1:A:310:MET:HE1	1.83	0.59
1:B:356:PRO:O	1:B:360:LEU:CD2	2.51	0.59
1:A:139:SER:H	1:A:142:HIS:HD2	1.47	0.59
1:A:208:ARG:NH2	1:A:248:LYS:O	2.36	0.59
1:B:79:GLN:HE22	1:B:83:GLN:CD	2.06	0.59
1:B:165:ARG:HG2	1:B:165:ARG:HH21	1.68	0.59
1:A:245:PHE:N	1:A:245:PHE:CD1	2.70	0.59
1:B:98:GLU:HG3	5:B:491:HOH:O	2.03	0.59
1:B:175:ASN:HD21	1:B:179:ASP:CB	2.15	0.59
1:B:342:ALA:O	1:B:343:GLU:HB3	2.03	0.58
1:A:53:TYR:CE1	1:A:84:ARG:NH1	2.67	0.58
1:A:154:LEU:HA	1:A:157:ILE:CG2	2.33	0.58
1:A:44:GLN:O	1:A:67:ARG:NH1	2.36	0.58
1:A:265:SER:OG	1:A:268:ASP:CB	2.32	0.58
1:A:31:VAL:O	1:A:31:VAL:CG2	2.52	0.58
1:B:306:LEU:HD22	1:B:310:MET:HE3	1.85	0.58
1:A:27:GLU:CD	1:A:28:VAL:N	2.54	0.58
1:A:142:HIS:CE1	5:A:385:HOH:O	2.57	0.58
1:B:61:ASP:OD2	1:B:104:ARG:NH2	2.36	0.58
1:B:70:ILE:HD11	1:B:119:TYR:CB	2.34	0.58
1:A:154:LEU:O	1:A:157:ILE:CG2	2.52	0.58
1:A:154:LEU:HD23	1:A:157:ILE:HG21	1.84	0.58
1:A:249:HIS:HB3	1:A:252:ASP:HB3	1.85	0.58
1:B:125:MET:HG3	1:B:173:LEU:HD23	1.85	0.57
1:B:328:PRO:CA	1:B:331:GLU:HG2	2.34	0.57
1:A:159:SER:HB3	1:A:341:VAL:HG22	1.72	0.57
1:A:96:ARG:HH21	1:A:96:ARG:HG3	1.70	0.57
1:B:108:ARG:NH2	1:B:365:PHE:CZ	2.73	0.57
1:A:51:GLY:C	1:A:53:TYR:N	2.54	0.57
1:B:205:VAL:HG23	5:B:521:HOH:O	2.04	0.57
1:B:351:GLU:HG3	5:B:445:HOH:O	2.05	0.57
1:A:349:ALA:HB3	1:A:352:LEU:CB	2.34	0.56
1:B:59:ALA:N	1:B:67:ARG:NH2	2.51	0.56
1:B:173:LEU:C	1:B:174:ILE:HG13	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:NE	1:A:61:ASP:OD1	2.36	0.56
1:A:61:ASP:OD2	1:A:64:ARG:HB2	2.06	0.56
1:A:63:VAL:HG23	1:A:64:ARG:N	2.20	0.56
1:A:370:ARG:HD3	1:B:193:PRO:HB3	1.87	0.56
1:B:34:GLN:HG3	1:B:55:MET:HE1	1.87	0.56
1:A:31:VAL:HG11	1:A:57:SER:OG	2.06	0.56
1:A:171:ASN:O	1:A:183:CYS:HB2	2.06	0.56
1:A:189:ARG:NH1	1:A:222:TYR:CE1	2.73	0.56
1:B:101:ILE:CD1	1:B:183:CYS:HA	2.24	0.56
1:B:244:ILE:O	1:B:245:PHE:HB2	2.06	0.56
1:A:242:ARG:HH21	1:A:242:ARG:CB	2.09	0.56
1:A:355:LEU:HD23	1:A:356:PRO:O	2.05	0.56
1:B:297:PRO:O	1:B:298:LYS:HB3	2.06	0.56
1:A:246:PRO:HB2	5:A:511:HOH:O	2.04	0.56
1:B:71:LYS:HG2	1:B:73:ILE:HD11	1.86	0.56
1:B:155:LYS:NZ	1:B:322:GLU:CD	2.58	0.56
1:A:61:ASP:OD2	1:A:64:ARG:NE	2.33	0.56
1:A:269:LEU:CD2	1:A:278:ARG:NH2	2.68	0.56
1:A:300:ASP:OD1	1:A:302:LYS:HB2	2.06	0.56
1:A:165:ARG:NH1	1:A:204:PTR:O3P	2.38	0.56
1:A:175:ASN:CG	1:A:179:ASP:HB2	2.26	0.56
1:A:268:ASP:O	1:A:269:LEU:C	2.41	0.56
1:A:270:ASN:CA	1:A:272:ILE:N	2.69	0.55
1:B:38:VAL:HG23	1:B:42:TYR:HB2	1.88	0.55
1:A:129:LEU:HD22	1:A:129:LEU:O	2.06	0.55
1:A:290:VAL:O	1:A:295:LEU:HD11	2.07	0.55
1:B:163:LEU:O	1:B:188:ALA:HA	2.07	0.55
1:A:217:LEU:HD12	1:A:277:ALA:HB1	1.88	0.55
1:A:322:GLU:OE1	1:A:322:GLU:HA	2.06	0.55
1:B:328:PRO:O	1:B:331:GLU:HG2	2.07	0.55
1:A:132:LEU:HD23	1:A:132:LEU:C	2.26	0.55
1:A:298:LYS:O	1:A:298:LYS:HG2	2.06	0.55
1:B:204:PTR:CE2	1:B:204:PTR:O3P	2.54	0.55
1:B:302:LYS:HE3	1:B:327:HIS:HE1	1.72	0.55
1:A:107:LEU:N	1:A:107:LEU:HD12	2.22	0.55
1:B:342:ALA:O	1:B:343:GLU:CG	2.54	0.55
1:A:175:ASN:HD21	1:A:179:ASP:CB	2.17	0.55
1:B:95:PHE:CE2	1:B:157:ILE:CD1	2.89	0.55
1:B:245:PHE:H	1:B:246:PRO:HD3	1.70	0.55
1:B:341:VAL:CG1	1:B:342:ALA:N	2.70	0.55
1:A:335:ASP:O	1:A:339:GLU:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ARG:NH1	1:B:63:VAL:HG22	2.21	0.54
1:B:175:ASN:HD21	1:B:179:ASP:CG	2.09	0.54
1:B:41:ARG:NH1	1:B:63:VAL:HG21	2.23	0.54
1:B:306:LEU:CD2	1:B:310:MET:CE	2.83	0.54
1:B:327:HIS:CE1	1:B:328:PRO:HD2	2.43	0.54
1:A:189:ARG:CZ	1:A:222:TYR:CE1	2.90	0.54
1:B:164:HIS:O	1:B:165:ARG:HB2	2.08	0.54
1:A:64:ARG:NH2	1:A:104:ARG:HG3	2.19	0.54
1:A:297:PRO:O	1:A:298:LYS:CB	2.56	0.54
1:A:350:MET:O	1:A:351:GLU:CG	2.55	0.54
1:B:177:THR:O	1:B:178:CYS:HB2	2.06	0.54
1:B:220:LYS:HE2	1:B:222:TYR:CE2	2.42	0.54
1:A:349:ALA:HB1	1:A:350:MET:C	2.28	0.54
1:A:349:ALA:HB1	1:A:351:GLU:N	2.23	0.54
1:A:154:LEU:HA	1:A:157:ILE:HG22	1.89	0.54
1:A:154:LEU:O	1:A:157:ILE:HG23	2.08	0.54
1:B:154:LEU:CA	1:B:157:ILE:HG22	2.38	0.54
1:A:244:ILE:HG23	1:A:245:PHE:CG	2.42	0.54
1:B:89:ILE:HD11	1:B:120:ILE:HD11	1.90	0.53
1:A:269:LEU:CD2	1:A:270:ASN:HD22	2.20	0.53
1:B:79:GLN:HB2	1:B:357:LYS:CD	2.27	0.53
1:A:106:ILE:HG21	1:A:368:THR:HG22	1.91	0.53
1:B:101:ILE:HD11	1:B:182:ILE:O	2.09	0.53
1:A:70:ILE:HD13	1:A:70:ILE:C	2.27	0.53
1:A:41:ARG:HD2	1:A:63:VAL:HG13	1.86	0.53
1:A:209:TRP:CD1	1:A:246:PRO:O	2.61	0.53
1:A:266:GLN:O	1:A:270:ASN:ND2	2.41	0.53
1:B:173:LEU:CD1	1:B:173:LEU:N	2.72	0.53
1:A:70:ILE:CD1	1:A:119:TYR:HD2	2.21	0.53
1:A:349:ALA:HA	5:B:479:HOH:O	2.08	0.53
1:B:41:ARG:HH11	1:B:63:VAL:CG2	2.22	0.53
1:B:101:ILE:CD1	1:B:182:ILE:O	2.57	0.53
1:A:64:ARG:O	1:A:65:LYS:CD	2.56	0.53
1:A:30:MET:HA	1:A:34:GLN:O	2.09	0.52
1:A:31:VAL:CG2	1:A:55:MET:SD	2.97	0.52
1:A:43:THR:O	1:A:44:GLN:HB2	2.10	0.52
1:A:75:PRO:O	1:A:76:PHE:HB2	2.09	0.52
1:A:244:ILE:HG12	1:A:245:PHE:CD1	2.44	0.52
1:B:180:LEU:C	1:B:180:LEU:HD23	2.29	0.52
1:A:107:LEU:HB2	1:A:119:TYR:HB2	1.91	0.52
1:B:203:GLU:CA	1:B:204:PTR:HD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLU:CG	1:A:28:VAL:N	2.72	0.52
1:B:218:ASN:HD22	1:B:219:SER:N	2.08	0.52
1:A:41:ARG:NH1	1:A:63:VAL:HG22	2.25	0.52
1:A:70:ILE:HD11	1:A:119:TYR:HD2	1.73	0.52
1:A:248:LYS:HB2	1:A:249:HIS:HB2	0.64	0.52
1:B:48:ILE:HB	1:B:56:VAL:HG22	1.91	0.52
1:A:350:MET:O	1:A:351:GLU:HG2	2.10	0.52
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.24	0.52
1:A:41:ARG:HD3	1:A:63:VAL:HG11	1.92	0.52
1:B:101:ILE:HD12	1:B:101:ILE:N	2.24	0.52
1:B:173:LEU:N	1:B:173:LEU:HD12	2.25	0.52
1:A:270:ASN:HA	1:A:272:ILE:H	1.73	0.52
1:A:351:GLU:OE1	1:B:270:ASN:OD1	2.28	0.52
1:B:128:ASP:HA	1:B:172:LEU:O	2.10	0.52
1:A:250:TYR:CD1	1:A:251:LEU:N	2.79	0.51
1:A:108:ARG:HH22	1:A:369:ALA:CA	2.24	0.51
1:B:292:TRP:HB3	1:B:304:LEU:HG	1.90	0.51
1:A:174:ILE:HA	1:A:179:ASP:O	2.10	0.51
1:A:296:PHE:N	1:A:297:PRO:HD3	2.25	0.51
1:A:199:GLY:HA2	1:A:274:ASN:ND2	2.26	0.51
1:A:235:LEU:HB3	1:A:307:LEU:HD23	1.91	0.51
1:A:53:TYR:CE2	1:A:184:ASP:HB3	2.45	0.51
1:B:58:SER:C	1:B:67:ARG:HH22	2.13	0.51
1:B:146:PHE:O	1:B:150:ILE:HG13	2.11	0.51
1:B:240:SER:HA	5:B:484:HOH:O	2.11	0.51
1:A:164:HIS:NE2	1:A:183:CYS:O	2.37	0.51
1:A:208:ARG:CZ	1:A:248:LYS:O	2.59	0.51
1:A:344:GLU:OE2	1:B:274:ASN:HB3	2.11	0.51
1:B:70:ILE:HD12	1:B:71:LYS:H	1.75	0.51
1:B:348:PHE:HB3	1:B:352:LEU:CD2	2.39	0.51
1:B:260:ILE:N	1:B:260:ILE:CD1	2.73	0.51
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.46	0.51
1:A:98:GLU:HG3	5:A:445:HOH:O	2.11	0.50
1:A:126:GLU:HG3	1:A:176:THR:N	2.25	0.50
1:B:160:ALA:HB2	1:B:342:ALA:CB	2.41	0.50
1:B:276:LYS:H	1:B:276:LYS:CE	2.23	0.50
1:A:27:GLU:C	1:A:28:VAL:HG22	2.32	0.50
1:A:334:TYR:CZ	1:A:336:PRO:HG3	2.46	0.50
1:A:358:GLU:OE1	1:A:361:LYS:CE	2.59	0.50
1:B:306:LEU:CD2	1:B:310:MET:HE3	2.41	0.50
1:B:53:TYR:OH	1:B:84:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LYS:HB3	5:B:509:HOH:O	2.09	0.50
1:A:248:LYS:H	1:A:248:LYS:HD2	1.77	0.50
1:B:160:ALA:HB2	1:B:342:ALA:HB2	1.93	0.50
1:B:260:ILE:O	1:B:290:VAL:HG22	2.11	0.50
1:A:139:SER:H	1:A:142:HIS:CD2	2.27	0.50
1:A:171:ASN:C	1:A:183:CYS:HB2	2.32	0.50
1:B:218:ASN:C	1:B:218:ASN:ND2	2.64	0.50
1:B:244:ILE:HG23	1:B:245:PHE:CD1	2.45	0.50
1:A:189:ARG:NH1	1:A:222:TYR:CZ	2.80	0.50
1:A:269:LEU:CB	1:A:270:ASN:HD22	2.24	0.50
1:A:351:GLU:HB2	5:A:419:HOH:O	2.11	0.50
1:B:244:ILE:O	1:B:245:PHE:CB	2.60	0.50
1:B:293:ALA:CB	1:B:294:LYS:NZ	2.75	0.50
1:A:248:LYS:CD	1:A:252:ASP:OD1	2.60	0.50
1:A:292:TRP:C	1:A:294:LYS:H	2.14	0.50
1:B:101:ILE:HG12	1:B:183:CYS:CB	2.41	0.50
1:A:334:TYR:HB2	5:A:411:HOH:O	2.11	0.49
1:B:268:ASP:O	1:B:271:CYS:HB3	2.11	0.49
1:B:325:LEU:HB3	1:B:334:TYR:CD1	2.48	0.49
1:A:312:THR:HG22	1:A:318:ARG:HG3	1.93	0.49
1:B:276:LYS:N	1:B:276:LYS:HZ3	2.10	0.49
1:B:314:ASN:ND2	1:B:314:ASN:C	2.64	0.49
1:B:108:ARG:NH1	1:B:365:PHE:O	2.46	0.49
1:B:356:PRO:O	1:B:360:LEU:HD22	2.12	0.49
1:A:28:VAL:HB	1:A:30:MET:HE3	1.93	0.49
1:B:83:GLN:OE1	1:B:353:ASP:CA	2.48	0.49
1:B:155:LYS:NZ	1:B:322:GLU:OE2	2.45	0.49
1:B:221:GLY:CA	1:B:226:ILE:HG13	2.34	0.49
1:A:125:MET:HG2	1:A:173:LEU:HB3	1.94	0.49
1:B:125:MET:O	4:B:382:5ID:H2	2.12	0.49
1:B:343:GLU:CG	1:B:344:GLU:N	2.72	0.49
1:A:248:LYS:N	1:A:249:HIS:HB3	2.28	0.49
1:A:165:ARG:HH12	1:A:204:PTR:P	2.36	0.49
1:A:249:HIS:HB3	1:A:252:ASP:CB	2.43	0.48
1:B:54:GLY:HA3	1:B:73:ILE:HD13	1.94	0.48
1:A:204:PTR:CD2	1:A:205:VAL:H	2.26	0.48
1:B:101:ILE:HD12	1:B:101:ILE:H	1.79	0.48
1:A:79:GLN:HA	1:A:357:LYS:HB3	1.94	0.48
1:A:240:SER:O	1:A:241:ASN:HB2	2.14	0.48
1:B:157:ILE:CD1	1:B:162:VAL:CB	2.84	0.48
1:B:157:ILE:HG23	1:B:158:HIS:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:PRO:HG2	1:B:359:ARG:HG3	1.95	0.48
1:A:106:ILE:HD12	1:A:371:PHE:CD2	2.48	0.48
1:A:197:HIS:O	1:A:220:LYS:HE3	2.13	0.48
1:A:269:LEU:HB3	1:A:272:ILE:HB	1.94	0.48
1:B:302:LYS:HE3	1:B:327:HIS:CE1	2.49	0.48
1:A:358:GLU:CD	1:A:361:LYS:HE2	2.33	0.48
1:B:95:PHE:CE1	1:B:346:PHE:HE1	2.32	0.48
1:B:290:VAL:HB	1:B:295:LEU:HD11	1.94	0.48
1:A:70:ILE:HD11	1:A:119:TYR:CD2	2.47	0.48
1:A:177:THR:O	1:A:178:CYS:HB2	2.13	0.48
1:A:349:ALA:CB	1:A:352:LEU:CG	2.92	0.48
1:B:89:ILE:HD11	1:B:120:ILE:CD1	2.44	0.48
1:B:155:LYS:HZ2	1:B:322:GLU:CD	2.15	0.48
1:B:249:HIS:CE1	1:B:252:ASP:HB2	2.49	0.48
1:A:41:ARG:NH1	1:A:63:VAL:CG2	2.77	0.47
1:B:32:LYS:CG	1:B:55:MET:SD	3.02	0.47
1:B:198:THR:HG21	1:B:220:LYS:HG2	1.94	0.47
1:B:363:LEU:O	1:B:367:GLU:HG2	2.14	0.47
1:A:325:LEU:HA	1:A:330:LEU:HD12	1.96	0.47
1:B:34:GLN:CG	1:B:55:MET:HE1	2.44	0.47
1:A:42:TYR:HA	1:A:60:TYR:O	2.14	0.47
1:A:146:PHE:O	1:A:150:ILE:HG13	2.14	0.47
1:A:151:LEU:HB2	1:A:325:LEU:HD21	1.96	0.47
1:A:154:LEU:O	1:A:157:ILE:HG22	2.15	0.47
1:A:270:ASN:O	1:A:270:ASN:OD1	2.32	0.47
1:B:358:GLU:CG	1:B:359:ARG:N	2.76	0.47
1:A:41:ARG:CD	1:A:63:VAL:CG1	2.77	0.47
1:A:41:ARG:CZ	1:A:63:VAL:HG21	2.44	0.47
1:B:245:PHE:N	1:B:246:PRO:CD	2.69	0.47
1:A:165:ARG:NE	1:A:189:ARG:HD3	2.29	0.47
1:A:248:LYS:HD2	1:A:248:LYS:N	2.29	0.47
1:B:168:LYS:O	1:B:172:LEU:HG	2.14	0.47
1:B:193:PRO:CD	1:B:194:GLU:OE1	2.62	0.47
1:A:24:VAL:N	1:A:25:PRO:CD	2.77	0.47
1:A:132:LEU:CD2	1:A:138:LEU:HD21	2.45	0.47
1:A:216:MET:HG3	1:A:254:LEU:HB2	1.96	0.47
1:A:349:ALA:CA	1:A:350:MET:CB	2.64	0.47
1:B:113:GLU:OE1	1:B:113:GLU:HA	2.14	0.47
1:B:360:LEU:HD22	1:B:360:LEU:N	2.29	0.47
1:A:189:ARG:CZ	1:A:189:ARG:HB3	2.43	0.47
1:A:375:VAL:HG21	1:B:323:GLU:OE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HG22	1:A:36:PHE:CE1	2.49	0.47
1:A:77:GLU:HB2	5:A:392:HOH:O	2.14	0.47
1:A:245:PHE:HE1	1:A:260:ILE:HD12	1.78	0.47
1:B:46:GLN:HB2	1:B:58:SER:HG	1.76	0.47
1:B:47:TYR:OH	1:B:50:GLU:HG2	2.15	0.47
1:B:358:GLU:O	1:B:362:GLU:HG3	2.14	0.47
1:A:204:PTR:CE2	1:A:205:VAL:HG12	2.45	0.47
1:A:173:LEU:C	1:A:174:ILE:HG13	2.35	0.46
1:A:250:TYR:O	1:A:251:LEU:CB	2.56	0.46
1:B:258:LEU:O	1:B:262:GLY:N	2.48	0.46
1:A:53:TYR:HE2	5:A:479:HOH:O	1.96	0.46
1:A:132:LEU:C	1:A:132:LEU:CD2	2.83	0.46
1:A:180:LEU:C	1:A:180:LEU:HD23	2.35	0.46
1:A:244:ILE:HG12	1:A:245:PHE:CZ	2.49	0.46
1:B:204:PTR:HE1	1:B:250:TYR:HD2	1.81	0.46
1:A:63:VAL:CG2	1:A:64:ARG:N	2.79	0.46
1:B:102:GLY:HA2	5:B:446:HOH:O	2.15	0.46
1:A:64:ARG:NH1	1:A:68:VAL:HG11	2.30	0.46
1:A:292:TRP:C	1:A:294:LYS:N	2.69	0.46
1:B:335:ASP:C	1:B:337:THR:H	2.18	0.46
1:A:154:LEU:CA	1:A:157:ILE:HG22	2.45	0.46
1:A:208:ARG:NH1	1:A:248:LYS:O	2.48	0.46
1:A:41:ARG:NE	1:A:63:VAL:CG2	2.79	0.46
1:A:94:ARG:CG	1:B:197:HIS:CD2	2.98	0.46
1:A:291:ALA:O	1:A:295:LEU:CD1	2.62	0.46
1:B:129:LEU:HD12	1:B:133:LEU:CG	2.42	0.46
1:B:145:TYR:CE2	1:B:149:GLN:NE2	2.83	0.46
1:B:154:LEU:HD11	1:B:227:ASP:HB3	1.97	0.46
1:B:306:LEU:CD2	1:B:310:MET:HE1	2.40	0.46
1:A:101:ILE:HG23	1:A:182:ILE:O	2.16	0.46
1:A:154:LEU:HD21	1:A:158:HIS:NE2	2.31	0.46
1:A:267:GLU:C	1:A:270:ASN:HB3	2.36	0.46
1:A:269:LEU:CB	1:A:270:ASN:HA	2.45	0.46
1:A:357:LYS:HA	1:A:360:LEU:HD12	1.98	0.46
1:B:174:ILE:HA	1:B:179:ASP:O	2.15	0.46
1:B:288:THR:HG22	1:B:289:LYS:N	2.31	0.46
1:A:58:SER:C	1:A:67:ARG:HH22	2.19	0.46
1:A:108:ARG:HG2	1:A:109:ALA:N	2.27	0.46
1:A:151:LEU:CB	1:A:325:LEU:HD21	2.45	0.46
1:B:45:LEU:N	1:B:45:LEU:CD1	2.79	0.46
1:B:145:TYR:CZ	1:B:149:GLN:NE2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLN:O	1:B:57:SER:CA	2.64	0.45
1:B:155:LYS:HD2	1:B:322:GLU:OE2	2.15	0.45
1:B:198:THR:CG2	1:B:219:SER:C	2.85	0.45
1:B:348:PHE:O	1:B:349:ALA:C	2.55	0.45
1:B:356:PRO:HG2	1:B:358:GLU:HG2	1.98	0.45
1:A:108:ARG:NH1	1:A:365:PHE:CE2	2.83	0.45
1:A:157:ILE:HG23	1:A:158:HIS:N	2.31	0.45
1:A:248:LYS:HD2	1:A:252:ASP:OD1	2.17	0.45
1:B:303:ALA:HB2	1:B:329:TYR:CE1	2.52	0.45
1:A:314:ASN:OD1	1:A:316:ASN:N	2.46	0.45
1:B:27:GLU:HG3	1:B:28:VAL:HG13	1.99	0.45
1:B:44:GLN:HE21	1:B:67:ARG:CZ	2.29	0.45
1:B:217:LEU:HD22	1:B:277:ALA:HB1	1.96	0.45
1:A:79:GLN:O	1:A:83:GLN:HG3	2.17	0.45
1:A:159:SER:OG	1:A:342:ALA:CB	2.64	0.45
1:B:191:ALA:O	1:B:192:ASP:HB3	2.16	0.45
1:B:314:ASN:HD22	1:B:315:PRO:N	2.13	0.45
1:A:76:PHE:CZ	1:A:115:MET:CE	3.00	0.45
1:A:156:TYR:O	1:A:159:SER:OG	2.27	0.45
1:B:154:LEU:HD23	1:B:157:ILE:HG21	1.98	0.45
1:B:195:HIS:ND1	5:B:497:HOH:O	2.34	0.45
1:B:306:LEU:HG	1:B:327:HIS:CG	2.52	0.45
1:B:314:ASN:HA	1:B:315:PRO:HD2	1.78	0.45
1:A:97:HIS:CD2	1:A:340:PRO:HG2	2.51	0.45
1:A:144:CYS:SG	1:A:333:TYR:HE2	2.39	0.45
1:A:96:ARG:HG3	1:A:96:ARG:NH2	2.32	0.45
1:A:208:ARG:CZ	1:A:249:HIS:N	2.80	0.45
1:B:88:GLU:HG3	1:B:185:PHE:HB2	1.99	0.45
1:A:53:TYR:OH	1:A:187:LEU:CD2	2.64	0.45
1:A:260:ILE:HG13	5:A:414:HOH:O	2.16	0.45
1:B:256:HIS:O	1:B:260:ILE:CD1	2.61	0.45
1:A:31:VAL:HG22	1:A:36:PHE:CD1	2.51	0.45
1:B:34:GLN:HG3	1:B:55:MET:HE3	1.96	0.45
1:B:46:GLN:O	1:B:57:SER:HA	2.17	0.45
1:B:131:LYS:HE3	5:B:469:HOH:O	2.16	0.45
1:A:26:GLY:O	1:A:27:GLU:HB3	2.17	0.44
1:B:173:LEU:O	1:B:180:LEU:HA	2.16	0.44
1:B:216:MET:HG3	1:B:250:TYR:CZ	2.52	0.44
1:B:243:PRO:HG2	1:B:246:PRO:HG3	1.99	0.44
1:A:189:ARG:CZ	1:A:189:ARG:CB	2.94	0.44
1:A:295:LEU:HD12	1:A:295:LEU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:THR:CG2	1:B:275:MET:HA	2.47	0.44
1:B:108:ARG:HD2	1:B:108:ARG:O	2.16	0.44
1:B:154:LEU:O	1:B:157:ILE:CG2	2.66	0.44
1:A:51:GLY:HA3	1:A:54:GLY:O	2.18	0.44
1:A:64:ARG:HD2	5:A:482:HOH:O	2.17	0.44
1:A:298:LYS:O	1:A:298:LYS:CG	2.63	0.44
1:B:90:GLN:OE1	1:B:367:GLU:OE1	2.36	0.44
1:B:95:PHE:HE1	1:B:346:PHE:CE1	2.35	0.44
1:B:97:HIS:HE1	1:B:99:ASN:OD1	2.00	0.44
1:B:166:ASP:OD2	1:B:206:ALA:HB1	2.17	0.44
1:A:101:ILE:HG12	1:A:101:ILE:O	2.17	0.44
1:B:79:GLN:CG	1:B:357:LYS:HD2	2.45	0.44
1:A:112:LEU:HD22	1:A:361:LYS:NZ	2.32	0.44
1:A:173:LEU:HD21	4:A:382:5ID:H2'	2.00	0.44
1:A:249:HIS:O	1:A:252:ASP:HB3	2.18	0.44
1:A:320:THR:H	1:A:323:GLU:CD	2.19	0.44
1:A:372:GLN:C	1:A:374:GLY:N	2.70	0.44
1:B:200:PHE:CD2	1:B:276:LYS:HB3	2.52	0.44
1:B:225:SER:HA	1:B:228:ILE:HD13	2.00	0.44
4:B:382:5ID:H5'1	4:B:382:5ID:H8	2.00	0.44
1:A:58:SER:HB2	1:A:124:LEU:HD11	1.99	0.44
1:A:208:ARG:HG3	1:A:253:GLN:OE1	2.18	0.44
1:B:46:GLN:O	1:B:57:SER:CB	2.63	0.44
1:A:165:ARG:HH22	1:A:204:PTR:CZ	2.31	0.44
1:A:307:LEU:HD11	1:A:311:LEU:HD12	2.00	0.44
1:A:120:ILE:N	1:A:120:ILE:CD1	2.74	0.43
1:A:245:PHE:HA	1:A:256:HIS:HB3	2.00	0.43
1:A:370:ARG:CD	1:B:193:PRO:HB3	2.46	0.43
1:B:360:LEU:HD22	1:B:360:LEU:H	1.83	0.43
1:A:36:PHE:CD2	1:A:45:LEU:CD2	2.99	0.43
1:A:60:TYR:CE2	1:A:62:HIS:CD2	3.06	0.43
1:A:312:THR:HG21	1:A:318:ARG:N	2.33	0.43
1:A:375:VAL:CG2	1:B:323:GLU:OE2	2.66	0.43
1:B:44:GLN:O	1:B:67:ARG:NH1	2.51	0.43
1:B:102:GLY:O	1:B:122:GLN:HG2	2.17	0.43
1:B:328:PRO:C	1:B:331:GLU:HG2	2.38	0.43
1:A:180:LEU:HD23	1:A:181:LYS:N	2.33	0.43
1:A:209:TRP:CD1	1:A:246:PRO:C	2.92	0.43
1:A:298:LYS:NZ	1:A:298:LYS:CB	2.69	0.43
1:B:125:MET:HG3	1:B:173:LEU:CB	2.48	0.43
1:A:372:GLN:C	1:A:374:GLY:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:CE1	1:B:346:PHE:CE1	3.06	0.43
1:B:95:PHE:CZ	1:B:157:ILE:HD12	2.52	0.43
1:B:165:ARG:NH2	1:B:165:ARG:HG2	2.33	0.43
1:B:201:LEU:HA	1:B:250:TYR:OH	2.18	0.43
1:A:292:TRP:HA	1:A:295:LEU:CD1	2.49	0.43
1:A:348:PHE:HE1	1:B:273:ILE:HG21	1.84	0.43
1:B:154:LEU:HA	1:B:154:LEU:HD23	1.85	0.43
1:B:290:VAL:HG21	1:B:295:LEU:HD21	2.01	0.43
1:B:76:PHE:CZ	1:B:115:MET:CE	3.01	0.43
1:B:276:LYS:O	1:B:277:ALA:C	2.57	0.43
1:B:314:ASN:HD21	1:B:316:ASN:HB2	1.84	0.43
1:A:64:ARG:HH22	1:A:104:ARG:CG	2.25	0.43
1:A:70:ILE:HD11	1:A:119:TYR:CB	2.49	0.43
1:B:155:LYS:NZ	1:B:322:GLU:OE1	2.51	0.43
1:B:341:VAL:HG12	1:B:342:ALA:N	2.34	0.43
1:A:76:PHE:CE2	1:A:361:LYS:HG3	2.54	0.43
1:A:171:ASN:HA	1:A:183:CYS:HB3	2.01	0.43
1:A:226:ILE:CG2	1:A:227:ASP:N	2.82	0.43
1:B:79:GLN:NE2	1:B:83:GLN:CD	2.71	0.43
1:A:47:TYR:CE2	1:A:49:GLY:HA2	2.54	0.43
1:B:172:LEU:HD11	1:B:234:ILE:HD13	2.01	0.43
1:B:205:VAL:HG11	5:B:547:HOH:O	2.19	0.43
1:B:208:ARG:CG	1:B:211:ARG:NH1	2.82	0.43
1:A:220:LYS:NZ	5:A:423:HOH:O	2.46	0.42
1:B:130:TYR:OH	1:B:134:LYS:HE2	2.19	0.42
1:B:245:PHE:HB3	1:B:253:GLN:HE22	1.84	0.42
1:A:65:LYS:CD	1:A:65:LYS:C	2.86	0.42
1:A:108:ARG:NH2	1:A:368:THR:OG1	2.52	0.42
1:A:248:LYS:N	1:A:249:HIS:CB	2.82	0.42
1:B:303:ALA:HB2	1:B:329:TYR:CZ	2.54	0.42
1:B:374:GLY:O	1:B:375:VAL:HG23	2.20	0.42
1:B:193:PRO:N	1:B:194:GLU:OE1	2.53	0.42
1:B:216:MET:HA	1:B:250:TYR:OH	2.20	0.42
1:A:108:ARG:HH22	1:A:369:ALA:N	2.17	0.42
1:A:267:GLU:CD	1:A:268:ASP:N	2.73	0.42
1:A:300:ASP:OD1	1:A:302:LYS:N	2.52	0.42
1:B:101:ILE:CG1	1:B:183:CYS:HB3	2.50	0.42
1:A:188:ALA:C	1:A:189:ARG:HG3	2.39	0.42
1:B:87:ARG:O	1:B:91:ILE:HG12	2.20	0.42
1:B:198:THR:OG1	1:B:199:GLY:N	2.53	0.42
1:A:213:PRO:O	1:A:217:LEU:HD23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD13	1:B:92:LEU:HA	1.76	0.42
1:B:159:SER:OG	1:B:341:VAL:HG13	2.20	0.42
1:B:278:ARG:NH1	5:B:479:HOH:O	2.53	0.42
1:B:338:ASP:HA	5:B:523:HOH:O	2.20	0.42
1:A:327:HIS:HA	1:A:328:PRO:HD3	1.90	0.42
1:B:86:LEU:HD11	1:B:367:GLU:HG3	2.02	0.42
1:B:352:LEU:N	5:B:460:HOH:O	2.52	0.42
1:A:36:PHE:CG	1:A:45:LEU:HD23	2.54	0.42
1:A:128:ASP:OD1	1:A:128:ASP:C	2.58	0.42
1:B:275:MET:CB	1:B:276:LYS:HZ1	2.26	0.42
1:B:304:LEU:HD12	1:B:304:LEU:HA	1.83	0.42
1:A:68:VAL:HA	1:A:124:LEU:HB2	2.02	0.42
1:A:163:LEU:O	1:A:188:ALA:HA	2.20	0.42
1:A:249:HIS:CG	1:A:252:ASP:CB	2.94	0.42
1:B:56:VAL:CG1	4:B:382:5ID:H5'2	2.49	0.42
1:A:79:GLN:OE1	1:A:83:GLN:CD	2.59	0.41
1:B:32:LYS:HB2	1:B:55:MET:HE1	2.02	0.41
1:B:87:ARG:HG3	1:B:348:PHE:CE2	2.54	0.41
1:B:154:LEU:C	1:B:157:ILE:HG22	2.39	0.41
1:B:194:GLU:OE1	1:B:194:GLU:N	2.31	0.41
1:B:334:TYR:CZ	1:B:336:PRO:HG3	2.55	0.41
1:A:157:ILE:HG23	1:A:158:HIS:H	1.84	0.41
1:B:154:LEU:HD13	1:B:158:HIS:CE1	2.55	0.41
1:B:207:THR:HG22	5:B:554:HOH:O	2.19	0.41
1:A:104:ARG:CZ	1:A:123:ASP:OD2	2.69	0.41
1:A:106:ILE:HG21	1:A:368:THR:CG2	2.48	0.41
1:A:246:PRO:HB2	1:A:247:GLY:H	1.73	0.41
1:A:59:ALA:CA	1:A:67:ARG:HH22	2.32	0.41
1:A:110:SER:HA	1:A:372:GLN:NE2	2.35	0.41
1:A:116:ARG:HG3	5:A:437:HOH:O	2.20	0.41
1:A:292:TRP:HA	1:A:295:LEU:HD12	2.01	0.41
1:A:182:ILE:CG2	1:A:183:CYS:N	2.83	0.41
1:B:101:ILE:CD1	1:B:101:ILE:H	2.32	0.41
1:B:292:TRP:O	1:B:296:PHE:N	2.42	0.41
1:A:51:GLY:O	1:A:52:ALA:C	2.59	0.41
1:A:309:ARG:HH21	1:A:309:ARG:HG2	1.85	0.41
1:A:355:LEU:CD2	1:A:356:PRO:O	2.68	0.41
1:A:372:GLN:OE1	1:A:372:GLN:HA	2.20	0.41
1:B:155:LYS:HZ3	1:B:322:GLU:CD	2.24	0.41
1:B:307:LEU:HD13	1:B:311:LEU:HD12	2.03	0.41
1:B:362:GLU:O	1:B:366:GLN:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:TYR:HE1	1:A:339:GLU:OE2	2.02	0.41
1:A:261:LEU:HD23	1:A:313:PHE:HB2	2.03	0.41
1:B:54:GLY:CA	1:B:73:ILE:HD13	2.51	0.41
1:B:211:ARG:CG	5:B:504:HOH:O	2.63	0.41
1:B:321:VAL:HG13	1:B:322:GLU:N	2.36	0.41
1:B:333:TYR:O	1:B:334:TYR:C	2.58	0.41
1:A:51:GLY:C	1:A:53:TYR:H	2.22	0.41
1:A:93:LEU:HD23	1:A:93:LEU:HA	1.93	0.41
1:A:106:ILE:HD12	1:A:371:PHE:CE2	2.55	0.41
1:A:215:ILE:HD11	1:A:226:ILE:HD11	2.03	0.41
1:A:269:LEU:HB3	1:A:270:ASN:HA	2.02	0.41
1:A:271:CYS:O	1:A:272:ILE:HD13	2.21	0.41
1:A:359:ARG:NH2	1:A:362:GLU:OE1	2.53	0.41
1:B:295:LEU:C	1:B:297:PRO:HD3	2.41	0.41
1:A:246:PRO:HD2	1:A:256:HIS:NE2	2.36	0.41
1:A:320:THR:CG2	1:A:323:GLU:OE2	2.68	0.41
1:B:264:PRO:HG2	1:B:269:LEU:HD21	2.03	0.41
1:A:269:LEU:CG	1:A:270:ASN:HD22	2.34	0.40
1:B:45:LEU:HA	1:B:58:SER:O	2.21	0.40
1:A:134:LYS:HE3	5:A:481:HOH:O	2.21	0.40
1:A:203:GLU:H	1:A:203:GLU:HG2	1.38	0.40
1:B:108:ARG:C	5:B:575:HOH:O	2.59	0.40
1:B:125:MET:CG	1:B:173:LEU:HB3	2.51	0.40
1:B:163:LEU:HD22	1:B:224:LYS:HA	2.02	0.40
1:B:226:ILE:HD13	1:B:226:ILE:HA	1.95	0.40
1:A:77:GLU:OE2	1:A:77:GLU:HA	2.21	0.40
1:A:139:SER:OG	1:A:142:HIS:CD2	2.74	0.40
1:B:203:GLU:CB	1:B:204:PTR:CG	2.99	0.40
1:B:296:PHE:HB2	1:B:304:LEU:HD21	2.03	0.40
1:A:76:PHE:CZ	1:A:115:MET:HE3	2.57	0.40
1:A:98:GLU:OE1	1:A:152:ARG:NH1	2.54	0.40
1:A:127:THR:HG23	1:A:128:ASP:N	2.35	0.40
1:A:250:TYR:HD1	1:A:251:LEU:N	2.19	0.40
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.77	0.40
1:A:349:ALA:CA	5:B:479:HOH:O	2.67	0.40
1:B:195:HIS:O	1:B:220:LYS:NZ	2.26	0.40
1:B:268:ASP:OD1	1:B:314:ASN:HB2	2.20	0.40
1:A:157:ILE:HB	5:A:412:HOH:O	2.21	0.40
1:A:350:MET:CE	1:B:278:ARG:HD3	2.52	0.40
1:B:70:ILE:HD11	1:B:119:TYR:CA	2.51	0.40
1:B:204:PTR:P	1:B:208:ARG:NH2	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASP:C	1:B:337:THR:N	2.75	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	349/382 (91%)	298 (85%)	34 (10%)	17 (5%)	2 1
1	B	349/382 (91%)	308 (88%)	29 (8%)	12 (3%)	3 3
All	All	698/764 (91%)	606 (87%)	63 (9%)	29 (4%)	3 2

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	GLU
1	A	184	ASP
1	A	191	ALA
1	A	249	HIS
1	A	269	LEU
1	A	270	ASN
1	B	191	ALA
1	B	205	VAL
1	B	206	ALA
1	B	343	GLU
1	A	30	MET
1	A	246	PRO
1	A	266	GLN
1	A	351	GLU
1	B	27	GLU
1	B	76	PHE
1	B	208	ARG

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Mol	Chain	Res	Type
1	A	32	LYS
1	A	53	TYR
1	A	75	PRO
1	A	298	LYS
1	B	342	ALA
1	B	26	GLY
1	B	218	ASN
1	B	250	TYR
1	A	192	ASP
1	A	28	VAL
1	B	245	PHE
1	A	245	PHE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	315/330 (96%)	282 (90%)	33 (10%)	7 9
1	B	315/330 (96%)	288 (91%)	27 (9%)	10 16
All	All	630/660 (96%)	570 (90%)	60 (10%)	8 12

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	36	PHE
1	A	56	VAL
1	A	65	LYS
1	A	70	ILE
1	A	80	THR
1	A	92	LEU
1	A	96	ARG
1	A	101	ILE
1	A	108	ARG
1	A	111	THR

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Mol	Chain	Res	Type
1	A	112	LEU
1	A	116	ARG
1	A	117	ASP
1	A	124	LEU
1	A	125	MET
1	A	128	ASP
1	A	129	LEU
1	A	154	LEU
1	A	183	CYS
1	A	203	GLU
1	A	216	MET
1	A	235	LEU
1	A	242	ARG
1	A	244	ILE
1	A	245	PHE
1	A	256	HIS
1	A	275	MET
1	A	295	LEU
1	A	304	LEU
1	A	322	GLU
1	A	347	THR
1	A	363	LEU
1	B	30	MET
1	B	56	VAL
1	B	70	ILE
1	B	75	PRO
1	B	92	LEU
1	B	101	ILE
1	B	113	GLU
1	B	117	ASP
1	B	126	GLU
1	B	129	LEU
1	B	132	LEU
1	B	154	LEU
1	B	194	GLU
1	B	198	THR
1	B	202	THR
1	B	218	ASN
1	B	251	LEU
1	B	276	LYS
1	B	294	LYS
1	B	304	LEU

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Mol	Chain	Res	Type
1	B	306	LEU
1	B	314	ASN
1	B	344	GLU
1	B	352	LEU
1	B	353	ASP
1	B	357	LYS
1	B	363	LEU

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

Mol	Chain	Res	Type
1	A	46	GLN
1	A	62	HIS
1	A	90	GLN
1	A	122	GLN
1	A	142	HIS
1	A	161	ASN
1	A	195	HIS
1	A	241	ASN
1	A	270	ASN
1	A	279	ASN
1	A	282	GLN
1	A	316	ASN
1	B	34	GLN
1	B	44	GLN
1	B	62	HIS
1	B	90	GLN
1	B	137	GLN
1	B	140	ASN
1	B	171	ASN
1	B	218	ASN
1	B	249	HIS
1	B	253	GLN
1	B	255	ASN
1	B	256	HIS
1	B	266	GLN
1	B	270	ASN
1	B	279	ASN
1	B	282	GLN
1	B	314	ASN
1	B	366	GLN
1	B	372	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
1	PTR	B	204	1	15,16,17	1.53	2 (13%)	19,22,24	1.65	5 (26%)
1	PTR	A	204	1	15,16,17	1.15	1 (6%)	19,22,24	1.65	4 (21%)

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
1	PTR	B	204	1	-	2/10/11/13	0/1/1/1
1	PTR	A	204	1	-	2/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	PTR	P-OH	-4.72	1.51	1.59
1	A	204	PTR	P-OH	-3.31	1.54	1.59
1	B	204	PTR	OH-CZ	-2.01	1.36	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	204	PTR	OH-P-O1P	-4.50	92.35	109.31
1	A	204	PTR	OH-P-O1P	-3.69	95.40	109.31
1	A	204	PTR	O3P-P-OH	-3.29	94.96	105.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	204	PTR	CG-CB-CA	-2.97	108.08	114.10
1	B	204	PTR	O3P-P-O2P	2.84	118.47	107.64
1	A	204	PTR	O3P-P-O2P	2.80	118.34	107.64
1	B	204	PTR	O3P-P-OH	-2.47	97.51	105.24
1	B	204	PTR	O2P-P-O1P	2.11	118.95	110.68
1	B	204	PTR	O3P-P-O1P	2.05	118.70	110.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	204	PTR	N-CA-CB-CG
1	A	204	PTR	C-CA-CB-CG
1	B	204	PTR	N-CA-CB-CG
1	B	204	PTR	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	204	PTR	14	0
1	A	204	PTR	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
4	5ID	B	382	-	20,22,22	1.35	2 (10%)	20,33,33	1.86	6 (30%)
4	5ID	A	382	-	20,22,22	1.25	2 (10%)	20,33,33	2.11	10 (50%)
2	SO4	A	380	-	4,4,4	0.50	0	6,6,6	0.45	0
2	SO4	B	380	-	4,4,4	0.62	0	6,6,6	0.16	0

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
4	5ID	B	382	-	-	0/2/22/22	0/3/3/3
4	5ID	A	382	-	-	0/2/22/22	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	382	5ID	C7-IAE	-4.15	2.02	2.10
4	A	382	5ID	C7-C5	3.89	1.47	1.42
4	B	382	5ID	C8-N9	-3.17	1.33	1.38
4	A	382	5ID	C7-IAE	-2.72	2.05	2.10

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	382	5ID	N3-C2-N1	-4.02	122.40	128.68
4	B	382	5ID	N3-C2-N1	-3.94	122.51	128.68
4	A	382	5ID	C2'-C3'-C4'	-3.49	95.86	102.64
4	B	382	5ID	O4'-C4'-C5'	3.42	116.60	109.21
4	B	382	5ID	C3'-C2'-C1'	3.32	105.97	100.98
4	A	382	5ID	C3'-C2'-C1'	3.31	105.96	100.98
4	A	382	5ID	C2-N1-C6	2.97	123.84	118.75
4	A	382	5ID	C7-C8-N9	2.52	110.99	108.22
4	B	382	5ID	C7-C8-N9	2.50	110.97	108.22
4	A	382	5ID	O2'-C2'-C3'	-2.49	103.76	111.82
4	A	382	5ID	C8-N9-C1'	2.42	127.63	125.48
4	B	382	5ID	O4'-C4'-C3'	2.33	109.72	105.11
4	A	382	5ID	O2'-C2'-C1'	-2.25	102.56	110.85
4	B	382	5ID	C2-N1-C6	2.20	122.52	118.75
4	A	382	5ID	C5'-C4'-C3'	-2.17	109.85	115.09
4	A	382	5ID	C5-C6-N1	-2.11	117.20	122.53

There are no chirality outliers.

There are no torsion outliers.

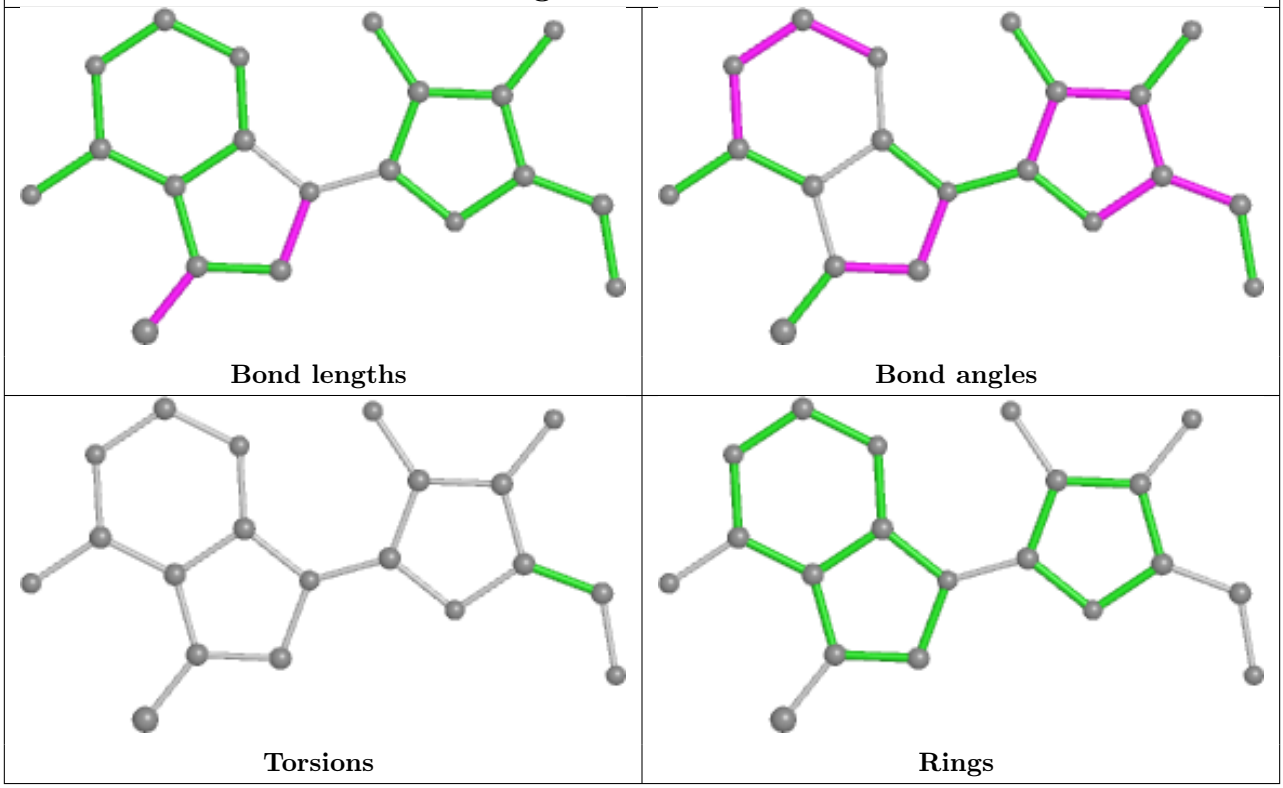
There are no ring outliers.

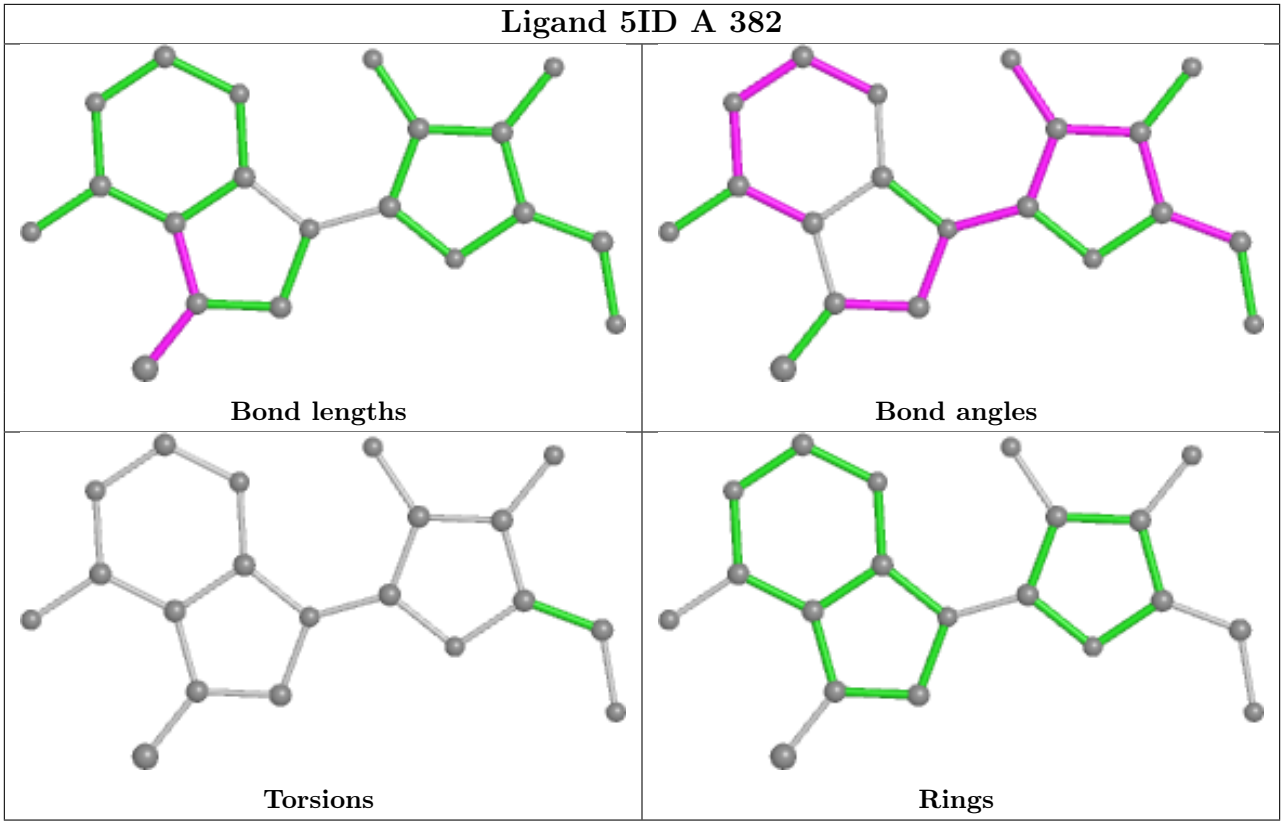
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	382	5ID	3	0
4	A	382	5ID	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 5ID B 382





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	351/382 (91%)	-0.02	10 (2%)	53	51	6, 20, 41, 71	0
1	B	351/382 (91%)	-0.12	12 (3%)	45	44	6, 19, 39, 81	0
All	All	702/764 (91%)	-0.07	22 (3%)	49	47	6, 19, 40, 81	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	VAL	9.3
1	A	375	VAL	5.3
1	B	26	GLY	5.0
1	B	24	VAL	4.9
1	A	53	TYR	4.6
1	A	374	GLY	4.5
1	B	25	PRO	4.5
1	B	374	GLY	4.3
1	B	205	VAL	4.0
1	A	25	PRO	3.6
1	B	53	TYR	3.5
1	B	352	LEU	3.2
1	B	350	MET	2.9
1	B	52	ALA	2.6
1	A	27	GLU	2.5
1	A	353	ASP	2.5
1	B	375	VAL	2.3
1	A	269	LEU	2.3
1	B	351	GLU	2.1
1	A	50	GLU	2.1
1	B	348	PHE	2.0
1	A	350	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PTR	A	204	16/17	0.80	0.28	30,45,48,49	0
1	PTR	B	204	16/17	0.84	0.24	34,40,43,44	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

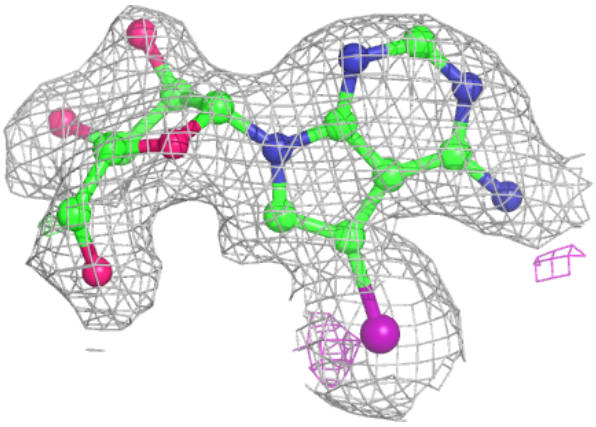
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

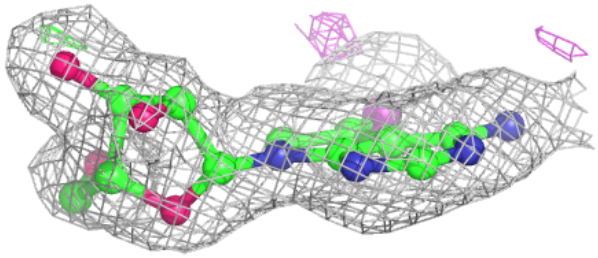
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	380	5/5	0.81	0.23	103,103,103,103	0
3	NA	A	381	1/1	0.92	0.38	41,41,41,41	0
2	SO4	A	380	5/5	0.96	0.12	33,36,37,40	0
3	NA	B	381	1/1	0.96	0.18	33,33,33,33	0
4	5ID	A	382	20/20	0.98	0.11	22,28,32,38	0
4	5ID	B	382	20/20	0.98	0.09	23,27,33,34	0

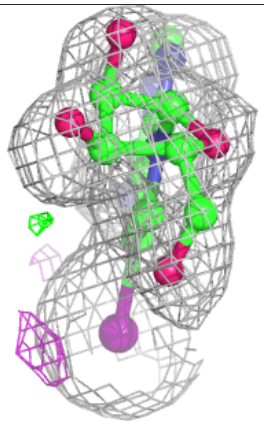
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 5ID A 382:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

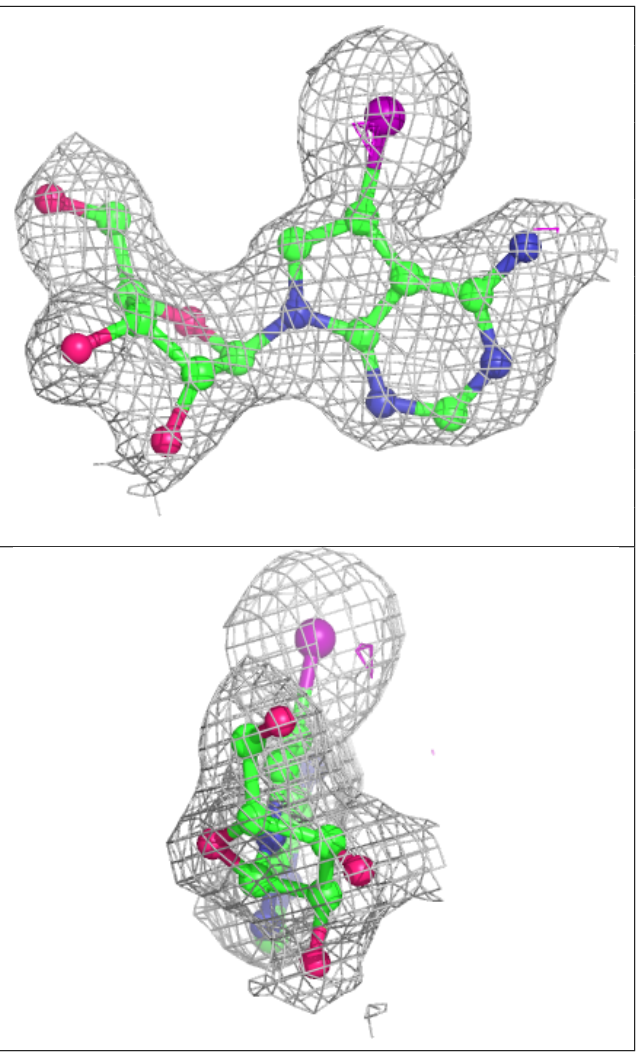






Electron density around 5ID B 382:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.