Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:10 AM GMT

PDB ID	:	2G01
Title	:	Pyrazoloquinolones as Novel, Selective JNK1 inhibitors
Authors	:	Abad-Zapatero, C.
Deposited on	:	2006-02-10
Resolution	:	3.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.50 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	Percentile Ranks	Value
Clashscore		64
Ramachandran outliers		13.1%
Sidechain outliers		10.7%

Worse　　　　　*Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
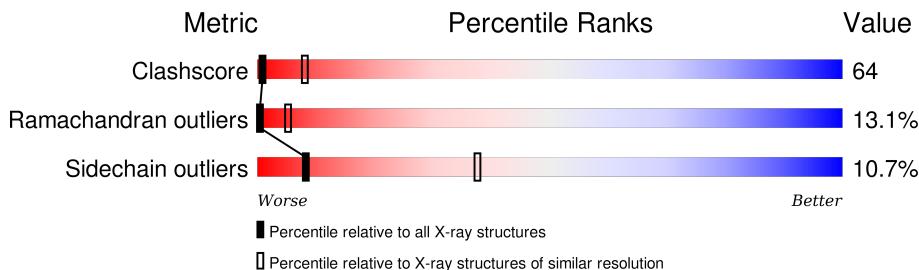
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	21% 58% 15% • •
1	B	370	29% 54% 13% • •
2	F	11	27% 45% 9% 9% 9%
2	G	11	64% 27% 9%
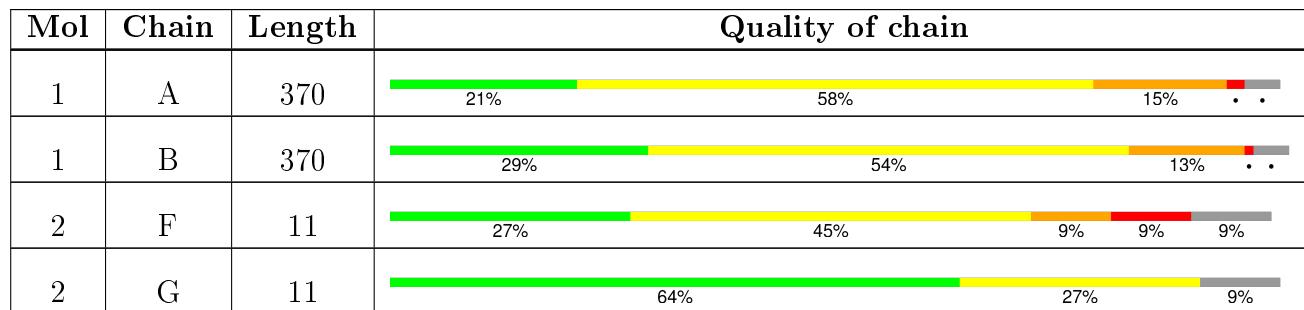
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5918 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 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total 2858	C 1834	N 482	O 520	S 22	0	0	1
1	B	357	Total 2858	C 1832	N 482	O 522	S 22	0	0	1

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	183	GLU	THR	ENGINEEERED	UNP P45983
A	185	GLU	TYR	ENGINEEERED	UNP P45983
A	365	HIS	-	EXPRESSION TAG	UNP P45983
A	366	HIS	-	EXPRESSION TAG	UNP P45983
A	367	HIS	-	EXPRESSION TAG	UNP P45983
A	368	HIS	-	EXPRESSION TAG	UNP P45983
A	369	HIS	-	EXPRESSION TAG	UNP P45983
A	370	HIS	-	EXPRESSION TAG	UNP P45983
B	183	GLU	THR	ENGINEEERED	UNP P45983
B	185	GLU	TYR	ENGINEEERED	UNP P45983
B	365	HIS	-	EXPRESSION TAG	UNP P45983
B	366	HIS	-	EXPRESSION TAG	UNP P45983
B	367	HIS	-	EXPRESSION TAG	UNP P45983
B	368	HIS	-	EXPRESSION TAG	UNP P45983
B	369	HIS	-	EXPRESSION TAG	UNP P45983
B	370	HIS	-	EXPRESSION TAG	UNP P45983

- Molecule 2 is a protein called C-jun-amino-terminal kinase-interacting protein 1.

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	10	Total 73	C 46	N 15	O 12	0	0	1
2	G	10	Total 73	C 46	N 15	O 12	0	0	1

• Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
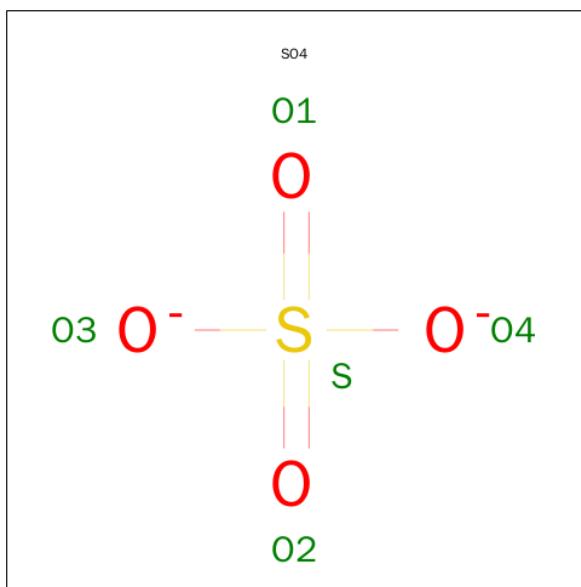
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

• Molecule 4 is 6-CHLORO-9-HYDROXY-1,3-DIMETHYL-1,9-DIHYDRO-4H-PYRAZOLO[
3,4-B]QUINOLIN-4-ONE (three-letter code: 73Q) (formula: $C_{12}H_{10}ClN_3O_2$).
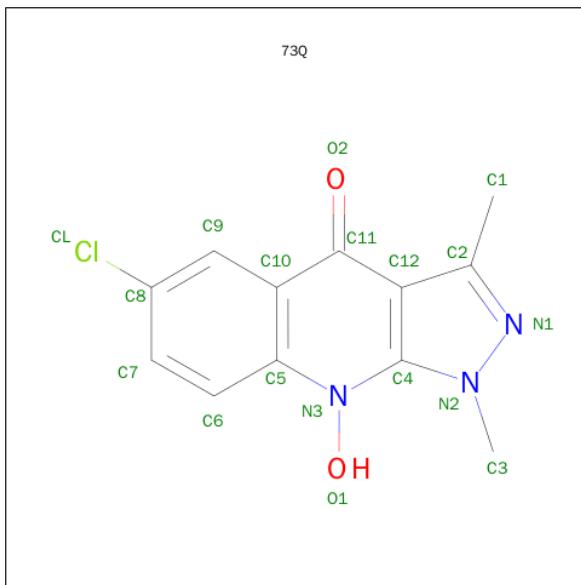
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			18	12	1	3	2		
4	B	1	Total	C	Cl	N	O	0	0
			18	12	1	3	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: Mitogen-activated protein kinase 8
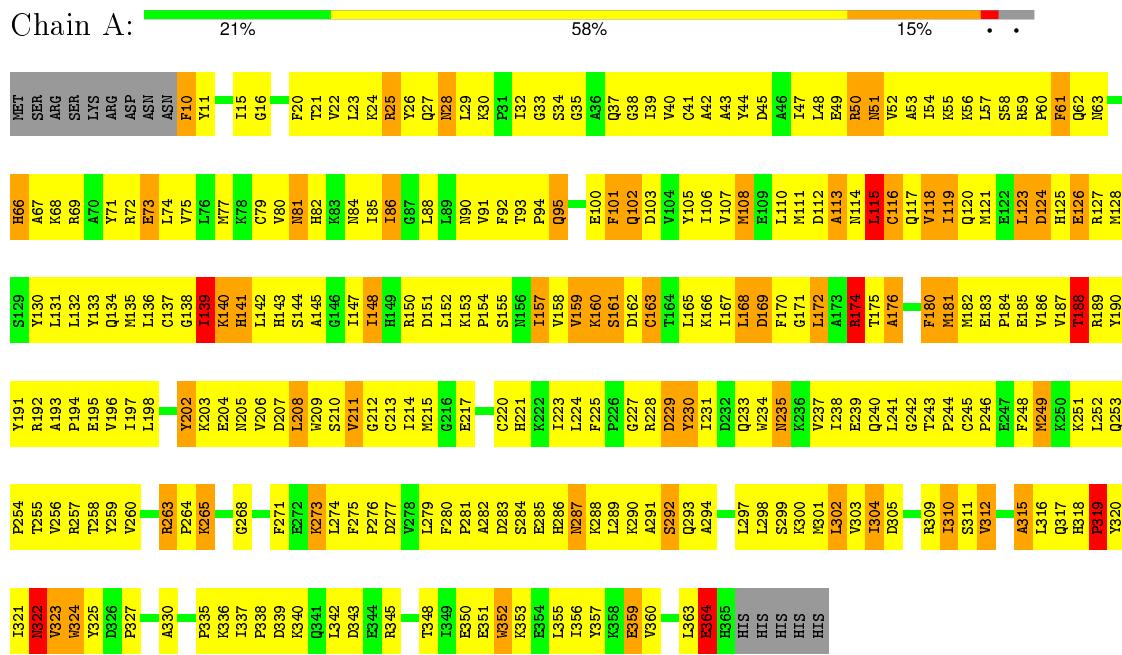
Chain A:

• Molecule 1: Mitogen-activated protein kinase 8

Chain B:

E272 K273 L274 F275 P276 D277 V278 L279 F280 P281 S284 E285 F286 N287 K290 Q293 A294 R295 D296 L297 L298 S299 K300 M301 L302 V303 I304 D305 A306 S307 K308 R309 I310 S311 V312 D313 E314 A315 L316 Q317 H318 P319 Y320 I321 N322 V323 W324 E329 A332 P333 P334 P335 K336 I337 P338

D339 K340 Q341 L342 D343 E344 R345 T348 I349 E350 E351 W352 K353 E354 L355 I356 Y357 K358 E359 D362 H365 HIS HIS HIS HIS HIS
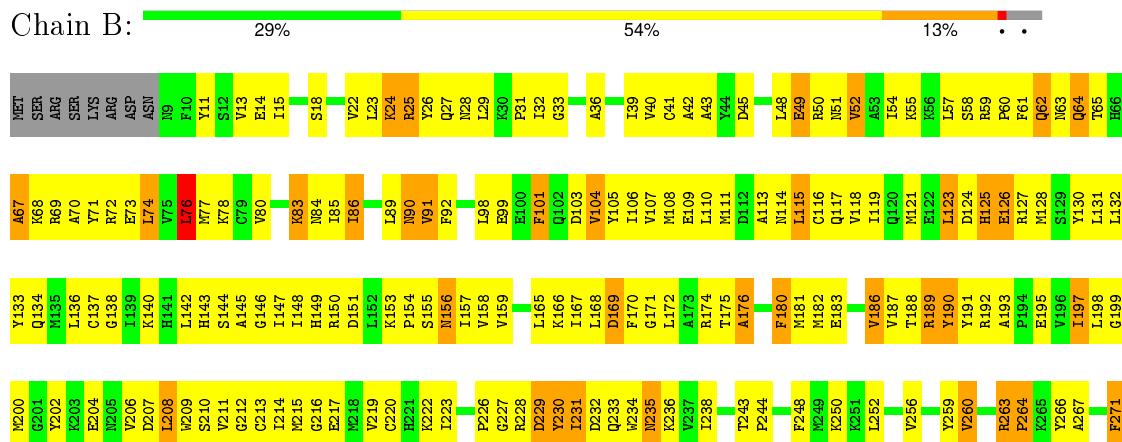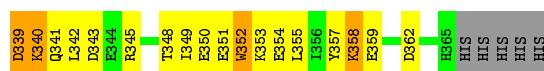
• Molecule 2: C-jun-amino-terminal kinase-interacting protein 1

Chain F:

| 27% | 45% | 9% | 9% | 9% |

ARG P554 K555 T558 T559 L560 N561 L562 F563

• Molecule 2: C-jun-amino-terminal kinase-interacting protein 1

Chain G:

| 64% | 27% | 9% |

ARG P554 K555 R556 L562 F563

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	150.62Å　150.62Å　119.00Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	19.89　–　3.50	Depositor
% Data completeness (in resolution range)	77.9 (19.89-3.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.283　,　0.354	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5918	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Full wwPDB X-ray Structure Validation Report

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: 73Q, SO4

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	0.39	0/2923	0.67	0/3956
1	B	0.41	0/2923	0.69	0/3959
2	F	0.62	0/74	0.87	0/100
2	G	0.58	0/74	0.75	0/100
All	All	0.41	0/5994	0.68	0/8115

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2858	0	2867	423	0
1	B	2858	0	2851	333	0
2	F	73	0	82	7	0
2	G	73	0	82	6	0
3	A	10	0	0	3	0
3	B	10	0	0	1	0
4	A	18	0	10	5	0
4	B	18	0	10	4	0
All	All	5918	0	5902	761	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 64.

All (761) 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:115:LEU:HD23	1:A:118:VAL:HG13	1.24	1.12
1:B:304:ILE:HD12	1:B:304:ILE:H	1.08	1.10
1:A:59:ARG:HH21	1:A:66:HIS:HB3	1.14	1.07
1:A:263:ARG:HA	1:A:263:ARG:HH11	1.16	1.06
1:A:115:LEU:HD12	1:A:157:ILE:HG21	1.40	1.04
1:A:263:ARG:NH1	1:A:264:PRO:HD3	1.74	1.02
1:B:348:THR:HB	1:B:351:GLU:H	1.27	0.98
1:A:235:ASN:HD21	1:A:263:ARG:NH2	1.61	0.97
1:A:128:MET:HG2	1:A:132:LEU:HD21	1.48	0.96
1:A:235:ASN:HD21	1:A:263:ARG:HH21	0.96	0.95
1:B:172:LEU:HD21	1:B:186:VAL:HG22	1.46	0.95
1:B:181:MET:HG3	1:B:202:TYR:HE2	1.30	0.95
1:B:57:LEU:HB2	1:B:104:VAL:HG23	1.48	0.94
1:A:142:LEU:H	1:A:142:LEU:HD22	1.32	0.93
1:B:304:ILE:CD1	1:B:304:ILE:H	1.79	0.93
1:B:271:PHE:O	1:B:295:ARG:HD3	1.69	0.92
1:B:318:HIS:ND1	1:B:319:PRO:HD2	1.84	0.92
1:B:51:ASN:HB3	1:B:110:LEU:HD23	1.52	0.91
1:B:215:MET:HE1	1:B:298:LEU:HB2	1.50	0.91
1:B:186:VAL:HG13	1:B:187:VAL:H	1.34	0.91
1:A:189:ARG:HA	1:A:192:ARG:HB2	1.49	0.91
1:A:115:LEU:HD23	1:A:118:VAL:CG1	2.01	0.90
1:A:72:ARG:HD3	1:A:174:ARG:HB3	1.51	0.90
1:A:323:VAL:HG23	1:A:324:TRP:H	1.37	0.89
1:A:263:ARG:HA	1:A:263:ARG:NH1	1.88	0.89
1:B:285:GLU:HG2	1:B:286:HIS:H	1.37	0.88
1:B:153:LYS:HD3	1:B:188:THR:HG21	1.53	0.88
1:B:132:LEU:HD11	1:B:215:MET:HG3	1.56	0.87
1:B:192:ARG:HH22	1:B:230:TYR:HB2	1.38	0.84
1:B:226:PRO:O	1:B:236:LYS:HG3	1.77	0.84
1:A:293:GLN:HG3	1:A:320:TYR:HB2	1.60	0.83
1:A:304:ILE:HD12	1:A:304:ILE:H	1.44	0.83
1:A:189:ARG:HB3	1:A:192:ARG:CZ	2.10	0.82
1:B:304:ILE:HD12	1:B:304:ILE:N	1.92	0.82
1:A:75:VAL:HG21	1:A:340:LYS:HD2	1.60	0.82
1:A:310:ILE:HG12	1:A:311:SER:H	1.42	0.82
1:B:54:ILE:HG12	1:B:107:VAL:HG22	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:HE3	1:A:292:SER:OG	1.80	0.81
1:B:115:LEU:O	1:B:115:LEU:HD23	1.81	0.81
1:A:59:ARG:HB3	1:A:66:HIS:ND1	1.96	0.80
1:B:181:MET:HG3	1:B:202:TYR:CE2	2.15	0.80
1:B:136:LEU:HB3	1:B:316:LEU:HD11	1.61	0.80
1:A:128:MET:HG2	1:A:132:LEU:CD2	2.11	0.80
1:B:285:GLU:HG2	1:B:286:HIS:N	1.96	0.79
1:A:115:LEU:HB2	1:A:157:ILE:HG22	1.64	0.79
1:A:198:LEU:HD13	1:A:252:LEU:HD21	1.65	0.79
1:A:32:ILE:HG13	1:A:33:GLY:N	1.96	0.79
1:A:111:MET:HB3	1:A:159:VAL:O	1.83	0.79
1:A:235:ASN:ND2	1:A:263:ARG:HH21	1.78	0.79
2:G:555:LYS:HD3	2:G:556:ARG:H	1.48	0.79
1:B:189:ARG:HA	1:B:192:ARG:HD3	1.65	0.78
1:B:227:GLY:HA3	1:B:233:GLN:NE2	1.98	0.78
1:A:174:ARG:HH11	1:A:176:ALA:HB2	1.49	0.77
1:A:115:LEU:C	1:A:117:GLN:H	1.87	0.77
1:B:271:PHE:CE1	1:B:299:SER:HA	2.19	0.77
1:B:189:ARG:NH1	1:B:229:ASP:HA	2.00	0.77
1:A:253:GLN:HB3	1:A:254:PRO:HD2	1.65	0.77
1:B:98:LEU:HD11	1:B:353:LYS:HG2	1.66	0.76
1:B:32:ILE:HG21	1:B:42:ALA:CB	2.16	0.76
1:B:150:ARG:HH21	1:B:181:MET:CG	1.98	0.76
1:A:113:ALA:HA	4:A:901:73Q:H33	1.67	0.76
1:B:136:LEU:HB3	1:B:316:LEU:CD1	2.16	0.75
1:B:172:LEU:HD21	1:B:186:VAL:CG2	2.15	0.75
1:B:132:LEU:O	1:B:136:LEU:HG	1.86	0.75
1:A:59:ARG:NH2	1:A:66:HIS:HB3	1.97	0.75
1:A:10:PHE:HB3	1:A:23:LEU:HA	1.67	0.75
1:B:297:LEU:HB2	1:B:318:HIS:CD2	2.21	0.74
1:B:90:ASN:ND2	1:B:91:VAL:H	1.86	0.73
1:B:32:ILE:HG21	1:B:42:ALA:HB3	1.71	0.73
1:A:125:HIS:HB3	1:A:289:LEU:HD23	1.70	0.73
1:A:38:GLY:HA2	1:A:58:SER:H	1.54	0.73
1:A:286:HIS:O	1:A:287:ASN:HB2	1.88	0.72
1:B:153:LYS:HD3	1:B:188:THR:CG2	2.19	0.72
1:A:318:HIS:HD2	1:A:319:PRO:HD2	1.54	0.72
1:B:148:ILE:HD11	1:B:204:GLU:HG2	1.71	0.72
1:B:217:GLU:OE1	1:B:223:ILE:HA	1.89	0.72
1:B:252:LEU:HD13	1:B:260:VAL:HG21	1.72	0.71
1:A:49:GLU:O	1:A:50:ARG:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:TYR:O	1:A:327:PRO:HD3	1.90	0.71
1:B:186:VAL:HG13	1:B:187:VAL:N	2.06	0.71
1:B:192:ARG:HH22	1:B:230:TYR:CB	2.04	0.71
1:A:208:LEU:HD13	1:A:311:SER:HA	1.73	0.70
1:A:142:LEU:CD2	1:A:142:LEU:H	2.05	0.70
1:B:180:PHE:CE2	1:B:199:GLY:HA2	2.26	0.70
1:A:118:VAL:HA	1:A:121:MET:HG3	1.73	0.70
1:A:223:ILE:N	1:A:223:ILE:HD12	2.07	0.70
1:B:116:CYS:O	1:B:119:ILE:HG12	1.91	0.70
1:A:297:LEU:HB2	1:A:318:HIS:HE1	1.56	0.70
1:B:136:LEU:HD13	1:B:315:ALA:HB1	1.74	0.70
1:B:279:LEU:H	1:B:279:LEU:HD12	1.56	0.70
1:B:285:GLU:CG	1:B:286:HIS:H	2.05	0.69
1:A:80:VAL:CG2	1:A:85:ILE:HG21	2.22	0.69
1:B:271:PHE:HZ	1:B:302:LEU:HB2	1.58	0.69
1:A:165:LEU:HD23	1:A:166:LYS:N	2.09	0.68
1:A:275:PHE:CE2	1:A:298:LEU:HD13	2.29	0.68
1:A:139:ILE:HD13	1:A:167:ILE:HD11	1.74	0.68
1:A:168:LEU:N	1:A:168:LEU:HD23	2.09	0.68
1:B:55:LYS:O	1:B:105:TYR:HA	1.93	0.68
1:B:310:ILE:HG13	1:B:314:GLU:HB2	1.74	0.68
1:A:180:PHE:HD1	1:A:181:MET:H	1.40	0.68
1:A:90:ASN:ND2	1:A:91:VAL:H	1.92	0.68
1:B:259:TYR:CE1	1:B:263:ARG:HD3	2.29	0.68
1:A:91:VAL:HG12	1:A:106:ILE:CD1	2.25	0.67
1:A:198:LEU:HD11	1:A:234:TRP:CH2	2.29	0.67
1:A:230:TYR:CE2	1:A:231:ILE:HG13	2.30	0.67
1:B:234:TRP:CE2	1:B:238:ILE:HG21	2.30	0.67
1:B:132:LEU:HD11	1:B:215:MET:CG	2.25	0.67
1:B:271:PHE:CD1	1:B:299:SER:HA	2.28	0.67
1:B:323:VAL:HG23	1:B:324:TRP:N	2.09	0.67
1:A:198:LEU:HD11	1:A:234:TRP:CZ3	2.30	0.67
1:A:244:PRO:HB2	1:A:248:PHE:CD2	2.29	0.67
1:A:273:LYS:HE2	1:A:273:LYS:HA	1.76	0.67
1:A:336:LYS:HG3	1:A:337:ILE:H	1.60	0.67
1:B:150:ARG:HH21	1:B:181:MET:HG2	1.59	0.66
2:G:555:LYS:HD3	2:G:556:ARG:N	2.09	0.66
1:B:290:LYS:HB2	1:B:293:GLN:HB2	1.78	0.66
1:B:11:TYR:OH	1:B:29:LEU:HD21	1.96	0.66
1:A:193:ALA:O	1:A:196:VAL:HB	1.95	0.66
1:B:145:ALA:HB3	1:B:147:ILE:HG13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:NE2	1:A:335:PRO:HD3	2.10	0.66
1:A:80:VAL:HG21	1:A:85:ILE:HG21	1.77	0.66
1:B:57:LEU:HD22	1:B:57:LEU:H	1.60	0.66
1:B:305:ASP:HB3	1:B:308:LYS:HE2	1.78	0.66
1:A:244:PRO:HB2	1:A:248:PHE:HD2	1.60	0.66
1:B:180:PHE:CD2	1:B:199:GLY:HA2	2.31	0.66
1:A:187:VAL:O	1:A:187:VAL:HG22	1.96	0.66
1:B:208:LEU:HD12	1:B:310:ILE:HG23	1.78	0.66
1:A:174:ARG:NH1	1:A:176:ALA:HB2	2.10	0.66
1:A:63:ASN:HB2	1:A:66:HIS:CD2	2.30	0.65
1:A:115:LEU:CD1	1:A:157:ILE:HG21	2.23	0.65
1:B:150:ARG:NH2	1:B:181:MET:HG2	2.12	0.65
1:A:56:LYS:HA	1:A:105:TYR:HA	1.78	0.65
1:B:15:ILE:HG22	1:B:15:ILE:O	1.97	0.65
1:B:150:ARG:NH2	1:B:181:MET:SD	2.67	0.65
1:B:192:ARG:HB3	1:B:197:ILE:HG22	1.79	0.65
1:B:137:CYS:HA	1:B:316:LEU:HD21	1.79	0.64
1:B:32:ILE:HD12	1:B:32:ILE:C	2.17	0.64
1:B:123:LEU:HD12	1:B:128:MET:HB2	1.78	0.64
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.62	0.64
1:A:172:LEU:H	1:A:172:LEU:HD23	1.62	0.64
1:A:115:LEU:HB2	1:A:157:ILE:CG2	2.28	0.64
1:A:157:ILE:HD11	1:A:167:ILE:HG12	1.79	0.64
1:B:145:ALA:HB2	1:B:335:PRO:HD2	1.78	0.64
1:B:63:ASN:O	1:B:65:THR:N	2.29	0.64
1:A:352:TRP:HA	1:A:352:TRP:CE3	2.33	0.64
1:A:91:VAL:HG12	1:A:106:ILE:HD12	1.80	0.64
1:B:318:HIS:CG	1:B:319:PRO:HD2	2.33	0.64
1:A:230:TYR:CD2	1:A:231:ILE:HG13	2.33	0.64
1:A:124:ASP:HA	1:A:281:PRO:HB3	1.79	0.63
1:B:86:ILE:HG13	1:B:168:LEU:HD11	1.79	0.63
1:A:309:ARG:O	1:A:310:ILE:O	2.17	0.63
1:A:316:LEU:HA	1:A:321:ILE:HG21	1.80	0.63
1:A:256:VAL:O	1:A:260:VAL:HG23	1.98	0.63
1:B:183:GLU:O	1:B:186:VAL:HG12	1.98	0.62
1:A:183:GLU:C	1:A:185:GLU:H	2.03	0.62
1:B:32:ILE:HD12	1:B:33:GLY:N	2.14	0.62
1:B:157:ILE:N	1:B:157:ILE:HD12	2.14	0.62
1:B:57:LEU:HD23	1:B:104:VAL:HG23	1.81	0.62
1:B:113:ALA:HA	4:B:1001:73Q:H33	1.79	0.62
1:B:352:TRP:HA	1:B:352:TRP:CE3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HD22	1:A:310:ILE:HG23	1.79	0.62
1:A:181:MET:HG3	1:A:183:GLU:H	1.65	0.62
1:A:115:LEU:N	1:A:157:ILE:O	2.24	0.62
1:B:146:GLY:HA2	1:B:204:GLU:OE2	2.00	0.62
1:A:74:LEU:O	1:A:77:MET:HB2	1.99	0.62
1:A:63:ASN:N	1:A:66:HIS:HE2	1.97	0.62
1:B:148:ILE:HD12	1:B:148:ILE:N	2.15	0.62
1:A:71:TYR:OH	1:A:340:LYS:HD3	1.99	0.62
1:A:143:HIS:ND1	1:A:312:VAL:HG21	2.15	0.62
1:B:60:PRO:O	1:B:67:ALA:HB2	2.00	0.62
1:A:318:HIS:CD2	1:A:319:PRO:HD2	2.33	0.62
1:A:84:ASN:O	1:A:166:LYS:HA	2.00	0.62
1:B:348:THR:HB	1:B:351:GLU:N	2.10	0.62
1:A:304:ILE:H	1:A:304:ILE:CD1	2.02	0.62
1:B:50:ARG:NH2	1:B:89:LEU:HD21	2.15	0.61
1:A:318:HIS:HD2	1:A:319:PRO:CD	2.14	0.61
1:B:227:GLY:HA3	1:B:233:GLN:HE22	1.64	0.61
1:B:149:HIS:O	1:B:150:ARG:HB2	2.01	0.61
1:B:57:LEU:HD11	1:B:106:ILE:HD11	1.83	0.61
1:B:123:LEU:O	1:B:281:PRO:HB3	1.99	0.61
1:A:38:GLY:HA2	1:A:58:SER:N	2.15	0.61
1:A:223:ILE:HG22	1:A:224:LEU:N	2.16	0.61
1:B:165:LEU:C	1:B:165:LEU:HD23	2.21	0.61
1:B:69:ARG:HB3	1:B:171:GLY:O	2.00	0.61
1:A:132:LEU:HD11	1:A:215:MET:HG2	1.82	0.61
1:A:80:VAL:O	1:A:81:ASN:HB2	2.01	0.61
1:B:150:ARG:HD3	1:B:172:LEU:O	2.00	0.61
1:B:114:ASN:O	1:B:116:CYS:N	2.34	0.61
1:B:312:VAL:O	1:B:316:LEU:HD13	2.01	0.61
1:A:220:CYS:O	1:A:221:HIS:HB2	2.01	0.60
1:A:128:MET:O	1:A:132:LEU:HD23	2.01	0.60
1:A:141:HIS:CE1	1:A:335:PRO:HD3	2.37	0.60
1:B:338:PRO:HG2	1:B:340:LYS:HG2	1.83	0.60
1:B:353:LYS:O	1:B:357:TYR:HB3	2.02	0.60
1:B:64:GLN:O	1:B:67:ALA:HB3	2.01	0.60
1:A:198:LEU:HD13	1:A:252:LEU:CD2	2.31	0.60
1:A:115:LEU:O	1:A:117:GLN:N	2.35	0.59
1:A:297:LEU:HB2	1:A:318:HIS:CE1	2.36	0.59
1:A:180:PHE:HD1	1:A:181:MET:N	2.00	0.59
1:B:169:ASP:O	1:B:170:PHE:HB2	2.01	0.59
1:B:219:VAL:O	1:B:279:LEU:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HG13	1:A:217:GLU:HG2	1.84	0.59
1:A:115:LEU:HD22	1:A:119:ILE:HD12	1.83	0.59
1:A:157:ILE:HD13	1:A:167:ILE:HA	1.85	0.59
1:A:158:VAL:HG22	1:A:168:LEU:HD22	1.84	0.59
1:A:112:ASP:O	1:A:113:ALA:HB2	2.03	0.59
1:A:125:HIS:O	1:A:126:GLU:C	2.41	0.59
1:B:341:GLN:C	1:B:343:ASP:H	2.05	0.59
1:A:22:VAL:HA	1:A:92:PHE:CZ	2.38	0.59
1:A:115:LEU:C	1:A:117:GLN:N	2.56	0.59
1:A:141:HIS:HB3	1:A:142:LEU:HD22	1.83	0.59
1:B:115:LEU:HB2	1:B:157:ILE:HB	1.84	0.59
1:A:215:MET:SD	1:A:297:LEU:HD23	2.43	0.58
1:A:142:LEU:N	1:A:142:LEU:HD22	2.11	0.58
1:A:186:VAL:HG13	1:A:187:VAL:N	2.18	0.58
1:B:86:ILE:HG13	1:B:168:LEU:CD1	2.33	0.58
1:A:134:GLN:NE2	1:A:163:CYS:O	2.33	0.58
1:A:202:TYR:O	1:A:202:TYR:CD1	2.56	0.58
1:A:10:PHE:HD2	1:A:23:LEU:CD2	2.17	0.58
1:A:119:ILE:CG1	1:A:217:GLU:HG2	2.34	0.58
1:A:234:TRP:NE1	1:A:238:ILE:HG21	2.18	0.58
1:A:22:VAL:HG12	1:A:92:PHE:HZ	1.68	0.58
1:B:23:LEU:O	1:B:25:ARG:N	2.36	0.58
1:A:139:ILE:HD13	1:A:167:ILE:CD1	2.33	0.58
1:B:147:ILE:C	1:B:148:ILE:HD12	2.24	0.58
1:A:350:GLU:O	1:A:353:LYS:HB3	2.03	0.58
1:A:248:PHE:O	1:A:251:LYS:HB2	2.03	0.58
1:A:208:LEU:HD22	1:A:310:ILE:CG2	2.34	0.58
1:A:231:ILE:HD12	1:B:259:TYR:CD2	2.38	0.58
1:A:95:GLN:HG2	1:A:100:GLU:O	2.03	0.58
1:A:352:TRP:O	1:A:356:ILE:HG13	2.03	0.58
1:B:197:ILE:HD11	1:B:234:TRP:HE3	1.69	0.57
1:A:252:LEU:HD12	1:A:252:LEU:N	2.19	0.57
1:A:301:MET:O	1:A:309:ARG:HG3	2.04	0.57
1:B:310:ILE:HG12	1:B:311:SER:N	2.19	0.57
1:A:68:LYS:HG3	1:A:352:TRP:HZ2	1.69	0.57
1:A:223:ILE:N	1:A:223:ILE:CD1	2.67	0.57
1:A:208:LEU:HD23	1:A:301:MET:HE3	1.85	0.57
1:B:275:PHE:CD1	1:B:298:LEU:HD21	2.40	0.57
1:B:153:LYS:CD	1:B:188:THR:HG21	2.29	0.57
1:A:32:ILE:HG12	1:A:40:VAL:O	2.05	0.57
1:A:45:ASP:OD2	1:A:48:LEU:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ALA:O	1:B:70:ALA:N	2.38	0.57
1:A:223:ILE:H	1:A:223:ILE:CD1	2.17	0.57
1:B:25:ARG:NH2	1:B:45:ASP:OD2	2.36	0.57
1:B:136:LEU:HD13	1:B:315:ALA:CB	2.34	0.57
1:A:183:GLU:O	1:A:186:VAL:HG12	2.05	0.57
1:B:315:ALA:C	1:B:317:GLN:H	2.09	0.56
1:B:297:LEU:HD13	1:B:318:HIS:CB	2.35	0.56
1:B:323:VAL:CG2	1:B:324:TRP:N	2.67	0.56
1:A:323:VAL:HG23	1:A:324:TRP:N	2.13	0.56
1:A:189:ARG:NE	3:A:501:SO4:S	2.73	0.56
1:A:353:LYS:HA	1:A:356:ILE:HD12	1.87	0.56
1:B:154:PRO:O	1:B:157:ILE:HD12	2.06	0.56
1:A:113:ALA:CA	4:A:901:73Q:H33	2.34	0.56
1:B:296:ASP:OD2	1:B:318:HIS:HE1	1.88	0.56
1:A:160:LYS:O	1:A:162:ASP:OD1	2.24	0.56
1:B:202:TYR:O	1:B:202:TYR:CD1	2.58	0.56
1:B:91:VAL:HG23	1:B:105:TYR:O	2.05	0.56
1:B:114:ASN:C	1:B:116:CYS:H	2.08	0.56
1:A:44:TYR:HB2	1:A:51:ASN:OD1	2.05	0.56
1:A:301:MET:O	1:A:303:VAL:N	2.38	0.56
1:A:176:ALA:HB3	1:A:202:TYR:CE1	2.41	0.56
1:A:304:ILE:O	1:A:305:ASP:C	2.44	0.56
1:B:167:ILE:HG22	1:B:168:LEU:N	2.21	0.56
1:A:315:ALA:O	1:A:318:HIS:HB3	2.06	0.56
1:B:165:LEU:HD23	1:B:166:LYS:N	2.21	0.56
1:A:125:HIS:O	1:A:127:ARG:N	2.39	0.55
1:B:229:ASP:OD1	1:B:232:ASP:N	2.39	0.55
1:B:214:ILE:HG22	1:B:215:MET:N	2.21	0.55
1:A:40:VAL:HA	1:A:54:ILE:O	2.06	0.55
1:A:271:PHE:HA	1:A:274:LEU:HB2	1.89	0.55
1:B:209:TRP:C	1:B:209:TRP:CD1	2.79	0.55
1:A:310:ILE:HG12	1:A:311:SER:N	2.17	0.55
1:A:237:VAL:CG1	1:A:238:ILE:N	2.70	0.55
1:A:108:MET:SD	4:A:901:73Q:H7	2.47	0.55
1:A:25:ARG:O	1:A:45:ASP:HA	2.07	0.55
1:A:242:GLY:N	1:A:268:GLY:HA2	2.22	0.55
1:B:354:GLU:O	1:B:358:LYS:N	2.39	0.55
1:A:264:PRO:O	1:A:265:LYS:O	2.24	0.55
1:B:303:VAL:O	1:B:309:ARG:NH2	2.35	0.55
1:A:50:ARG:O	1:A:52:VAL:HG13	2.06	0.55
1:B:25:ARG:HG2	1:B:26:TYR:CD2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:TYR:HA	1:A:51:ASN:HA	1.88	0.55
1:B:197:ILE:HD11	1:B:234:TRP:CE3	2.42	0.55
1:B:352:TRP:HE3	1:B:352:TRP:HA	1.71	0.55
1:B:216:GLY:CA	1:B:298:LEU:HD11	2.37	0.54
1:B:300:LYS:O	1:B:310:ILE:HG22	2.07	0.54
1:B:323:VAL:HG23	1:B:324:TRP:CD2	2.42	0.54
1:A:68:LYS:HB2	1:A:352:TRP:HE1	1.72	0.54
1:A:242:GLY:H	1:A:268:GLY:HA2	1.71	0.54
1:A:125:HIS:O	1:A:128:MET:N	2.41	0.54
1:B:303:VAL:HB	1:B:309:ARG:HB2	1.90	0.54
1:B:357:TYR:O	1:B:359:GLU:N	2.41	0.54
1:B:15:ILE:HD12	1:B:31:PRO:HG3	1.88	0.54
1:A:114:ASN:HA	1:A:158:VAL:HA	1.90	0.54
1:B:275:PHE:HB3	1:B:280:PHE:CE2	2.43	0.54
1:B:52:VAL:HA	1:B:110:LEU:HB2	1.89	0.54
1:A:243:THR:HG23	1:A:244:PRO:HD2	1.89	0.54
1:A:169:ASP:C	1:A:170:PHE:HD1	2.11	0.54
1:B:348:THR:HB	1:B:351:GLU:HB2	1.89	0.54
1:B:39:ILE:HD12	1:B:39:ILE:N	2.22	0.54
1:B:39:ILE:O	1:B:55:LYS:HA	2.07	0.54
1:A:189:ARG:NE	3:A:501:SO4:O2	2.39	0.54
1:A:195:GLU:H	1:A:195:GLU:CD	2.12	0.54
1:A:304:ILE:N	1:A:304:ILE:HD12	2.19	0.54
1:A:263:ARG:HH12	1:A:264:PRO:HD3	1.69	0.53
1:B:158:VAL:HG23	1:B:166:LYS:HB2	1.90	0.53
1:A:212:GLY:C	1:A:214:ILE:N	2.61	0.53
1:B:202:TYR:O	1:B:202:TYR:HD1	1.92	0.53
1:B:339:ASP:O	1:B:341:GLN:HG3	2.09	0.53
1:B:296:ASP:HB3	1:B:318:HIS:NE2	2.24	0.53
1:B:212:GLY:O	1:B:302:LEU:HD21	2.07	0.53
1:B:136:LEU:CD1	1:B:315:ALA:HB1	2.37	0.53
1:A:32:ILE:CG1	1:A:33:GLY:N	2.68	0.53
1:B:256:VAL:O	1:B:259:TYR:HB3	2.09	0.53
1:A:225:PHE:CE1	1:A:237:VAL:HG23	2.44	0.53
1:A:39:ILE:O	1:A:55:LYS:HA	2.08	0.53
1:B:72:ARG:O	1:B:76:LEU:HB2	2.09	0.53
1:B:189:ARG:NH1	1:B:229:ASP:CA	2.71	0.53
1:B:113:ALA:O	1:B:159:VAL:HG22	2.07	0.53
1:A:157:ILE:O	1:A:157:ILE:HG22	2.08	0.53
1:B:192:ARG:NH2	1:B:230:TYR:HB2	2.18	0.53
1:B:32:ILE:HG23	1:B:42:ALA:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:HB3	1:A:206:VAL:HG23	1.91	0.53
1:A:298:LEU:HD22	1:A:302:LEU:HG	1.89	0.53
1:A:310:ILE:HG23	1:A:311:SER:N	2.22	0.53
1:B:278:VAL:C	1:B:280:PHE:N	2.60	0.53
1:B:117:GLN:HE21	2:G:562:LEU:HB3	1.74	0.53
1:A:124:ASP:O	1:A:125:HIS:HB2	2.08	0.53
1:B:348:THR:CB	1:B:351:GLU:HB2	2.39	0.53
1:A:237:VAL:HG13	1:A:238:ILE:N	2.24	0.53
1:B:114:ASN:OD1	1:B:116:CYS:CB	2.57	0.52
1:A:131:LEU:CD2	1:A:165:LEU:HD12	2.39	0.52
1:A:208:LEU:HD11	1:A:312:VAL:N	2.24	0.52
1:A:298:LEU:O	1:A:301:MET:N	2.34	0.52
1:A:208:LEU:CD1	1:A:311:SER:HA	2.38	0.52
1:A:352:TRP:HA	1:A:352:TRP:HE3	1.72	0.52
1:B:156:ASN:OD1	1:B:169:ASP:HB2	2.09	0.52
1:B:296:ASP:C	1:B:298:LEU:H	2.11	0.52
1:B:309:ARG:O	1:B:310:ILE:O	2.27	0.52
1:B:354:GLU:OE2	1:B:358:LYS:HD2	2.08	0.52
1:B:296:ASP:O	1:B:300:LYS:N	2.41	0.52
1:A:181:MET:C	1:A:183:GLU:H	2.11	0.52
1:B:208:LEU:HD12	1:B:310:ILE:CG2	2.38	0.52
1:B:157:ILE:HG21	1:B:165:LEU:HD11	1.91	0.52
1:A:157:ILE:CD1	1:A:167:ILE:HA	2.40	0.52
1:A:115:LEU:HD12	1:A:157:ILE:CG2	2.27	0.52
1:B:140:LYS:HA	1:B:312:VAL:HG21	1.92	0.52
1:A:112:ASP:HB2	1:A:160:LYS:HA	1.92	0.51
1:B:64:GLN:HG3	1:B:349:ILE:HG22	1.91	0.51
1:B:148:ILE:HG22	1:B:150:ARG:HG3	1.92	0.51
1:A:101:PHE:HD1	1:A:102:GLN:N	2.09	0.51
1:B:50:ARG:HH21	1:B:89:LEU:HD11	1.75	0.51
1:A:29:LEU:O	1:A:30:LYS:HD3	2.09	0.51
1:B:175:THR:O	1:B:176:ALA:O	2.28	0.51
1:A:298:LEU:HD22	1:A:302:LEU:CD1	2.40	0.51
1:B:92:PHE:CE1	1:B:105:TYR:HB2	2.45	0.51
1:A:95:GLN:HG2	1:A:100:GLU:C	2.31	0.51
1:A:93:THR:O	1:A:93:THR:HG23	2.11	0.51
1:B:198:LEU:HD13	1:B:252:LEU:HD22	1.93	0.51
1:B:73:GLU:HG2	1:B:77:MET:HE2	1.92	0.51
1:A:290:LYS:HE3	1:A:292:SER:HG	1.76	0.51
1:A:234:TRP:CE2	1:A:238:ILE:HG21	2.45	0.51
1:A:287:ASN:OD1	1:A:288:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD23	1:B:104:VAL:CG2	2.39	0.51
1:B:80:VAL:HG11	1:B:85:ILE:HD13	1.91	0.51
1:A:142:LEU:HB3	1:A:147:ILE:HB	1.92	0.51
1:A:291:ALA:O	1:A:293:GLN:N	2.43	0.51
1:A:195:GLU:CD	1:A:309:ARG:HH22	2.14	0.51
1:A:322:ASN:O	1:A:323:VAL:C	2.49	0.51
1:B:143:HIS:HB2	1:B:312:VAL:HG11	1.92	0.51
1:A:181:MET:C	1:A:183:GLU:N	2.65	0.51
1:A:115:LEU:HA	1:A:118:VAL:CG1	2.41	0.51
1:A:138:GLY:O	1:A:139:ILE:C	2.50	0.51
1:B:316:LEU:N	1:B:316:LEU:HD12	2.26	0.51
1:A:208:LEU:O	1:A:209:TRP:C	2.48	0.50
1:A:318:HIS:CD2	1:A:319:PRO:CD	2.94	0.50
1:B:337:ILE:HG23	1:B:338:PRO:HD2	1.93	0.50
1:A:79:CYS:O	1:A:335:PRO:HB2	2.12	0.50
1:B:357:TYR:C	1:B:359:GLU:H	2.14	0.50
1:A:56:LYS:O	1:A:57:LEU:HB2	2.11	0.50
1:A:209:TRP:O	1:A:210:SER:C	2.49	0.50
1:A:184:PRO:C	1:A:186:VAL:H	2.13	0.50
1:B:154:PRO:O	1:B:156:ASN:N	2.45	0.50
1:A:108:MET:SD	4:A:901:73Q:CL	3.07	0.50
1:A:337:ILE:C	1:A:337:ILE:HD12	2.32	0.50
1:A:189:ARG:HB3	1:A:192:ARG:NH2	2.24	0.50
1:A:255:THR:HG23	3:B:701:SO4:O4	2.12	0.50
1:A:254:PRO:HG2	1:A:255:THR:H	1.76	0.50
1:A:25:ARG:HD2	1:A:47:ILE:HG21	1.92	0.50
1:A:293:GLN:HG3	1:A:320:TYR:CB	2.37	0.50
1:A:311:SER:O	1:A:315:ALA:HB2	2.12	0.50
1:A:21:THR:HB	1:A:94:PRO:HB3	1.92	0.50
1:A:126:GLU:HA	1:A:324:TRP:HH2	1.77	0.50
1:A:153:LYS:HB2	1:A:154:PRO:HD2	1.94	0.50
1:A:287:ASN:C	1:A:289:LEU:H	2.14	0.50
1:A:35:GLY:HA3	1:A:38:GLY:O	2.11	0.50
1:A:47:ILE:O	1:A:47:ILE:HG13	2.12	0.50
1:A:312:VAL:O	1:A:315:ALA:HB3	2.12	0.50
1:B:275:PHE:CE1	1:B:298:LEU:HD21	2.46	0.50
1:A:252:LEU:HD12	1:A:252:LEU:H	1.75	0.50
1:A:245:CYS:O	1:A:248:PHE:HB3	2.11	0.50
1:A:128:MET:O	1:A:132:LEU:CD2	2.60	0.49
1:A:254:PRO:O	1:A:257:ARG:HB3	2.12	0.49
1:B:271:PHE:CZ	1:B:302:LEU:HB2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PHE:O	1:A:181:MET:HB2	2.12	0.49
1:A:72:ARG:NH1	1:A:174:ARG:HG2	2.26	0.49
1:B:70:ALA:O	1:B:74:LEU:HB2	2.12	0.49
1:B:167:ILE:CG2	1:B:168:LEU:N	2.74	0.49
1:B:73:GLU:HB2	1:B:171:GLY:HA2	1.95	0.49
1:B:310:ILE:CG1	1:B:314:GLU:HB2	2.39	0.49
1:A:187:VAL:O	1:A:188:THR:C	2.49	0.49
1:A:61:PHE:CE1	1:A:353:LYS:HE2	2.47	0.49
1:A:88:LEU:HD21	1:A:91:VAL:CG1	2.42	0.49
1:B:259:TYR:OH	1:B:263:ARG:NE	2.45	0.49
1:B:48:LEU:O	1:B:49:GLU:HB2	2.11	0.49
1:A:128:MET:C	1:A:132:LEU:HD23	2.33	0.49
1:A:163:CYS:HA	2:F:560:LEU:HD22	1.93	0.49
1:B:234:TRP:CE2	1:B:238:ILE:CG2	2.95	0.49
1:B:25:ARG:HG2	1:B:26:TYR:CE2	2.48	0.49
1:A:172:LEU:HD23	1:A:172:LEU:N	2.28	0.49
1:A:211:VAL:O	1:A:214:ILE:HB	2.13	0.49
1:B:216:GLY:O	1:B:220:CYS:HB2	2.13	0.49
1:A:107:VAL:O	1:A:108:MET:HB3	2.12	0.49
1:B:29:LEU:HD22	1:B:29:LEU:N	2.28	0.49
1:A:189:ARG:HB3	1:A:192:ARG:NE	2.28	0.49
1:A:27:GLN:O	1:A:28:ASN:C	2.51	0.49
1:A:194:PRO:HD3	1:A:209:TRP:CE2	2.48	0.49
1:A:260:VAL:O	1:A:263:ARG:HG2	2.12	0.49
1:B:319:PRO:HA	1:B:322:ASN:OD1	2.12	0.49
1:B:167:ILE:C	1:B:168:LEU:HD22	2.33	0.49
1:A:160:LYS:O	1:A:160:LYS:HG2	2.13	0.49
1:A:119:ILE:HG22	1:A:120:GLN:HG2	1.95	0.48
1:B:86:ILE:HG21	1:B:108:MET:SD	2.52	0.48
1:A:363:LEU:HD12	1:A:363:LEU:N	2.28	0.48
1:A:94:PRO:HG3	1:A:105:TYR:CE1	2.47	0.48
1:A:183:GLU:C	1:A:185:GLU:N	2.64	0.48
1:A:193:ALA:CB	1:A:206:VAL:HG23	2.43	0.48
1:B:125:HIS:O	1:B:126:GLU:C	2.49	0.48
1:A:135:MET:O	1:A:139:ILE:CD1	2.61	0.48
1:A:135:MET:O	1:A:139:ILE:HG12	2.14	0.48
1:B:274:LEU:HB2	1:B:275:PHE:CD2	2.49	0.48
1:A:325:TYR:HE1	1:A:330:ALA:HB1	1.78	0.48
1:B:68:LYS:O	1:B:71:TYR:HB3	2.13	0.48
1:B:80:VAL:HG11	1:B:85:ILE:CD1	2.44	0.48
2:F:554:PRO:O	2:F:555:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:LEU:CD2	1:B:345:ARG:HD3	2.42	0.48
1:A:174:ARG:CZ	1:A:343:ASP:HB3	2.44	0.48
1:A:154:PRO:HD3	1:A:214:ILE:HD13	1.95	0.48
1:A:263:ARG:N	1:A:263:ARG:HD2	2.26	0.48
1:A:174:ARG:HB2	1:A:343:ASP:OD1	2.14	0.48
1:B:114:ASN:OD1	1:B:116:CYS:HB2	2.13	0.48
1:A:208:LEU:HD23	1:A:301:MET:CE	2.42	0.48
1:B:11:TYR:HD1	1:B:24:LYS:HA	1.78	0.48
1:A:107:VAL:HG12	1:A:108:MET:N	2.28	0.48
1:A:162:ASP:HB2	2:F:558:THR:O	2.14	0.48
1:B:332:ALA:HB1	1:B:333:PRO:HD2	1.94	0.48
2:F:561:ASN:C	2:F:561:ASN:HD22	2.16	0.48
1:A:142:LEU:HB3	1:A:147:ILE:CG2	2.43	0.48
1:A:85:ILE:CD1	1:A:167:ILE:HB	2.44	0.48
1:B:317:GLN:HA	1:B:317:GLN:OE1	2.14	0.48
1:A:318:HIS:C	1:A:318:HIS:CD2	2.87	0.48
1:A:62:GLN:N	1:A:66:HIS:HE2	2.12	0.47
1:B:187:VAL:HG13	1:B:192:ARG:CG	2.44	0.47
1:A:32:ILE:HG12	1:A:40:VAL:HG13	1.96	0.47
1:B:108:MET:SD	4:B:1001:73Q:CL	3.09	0.47
1:A:170:PHE:CD1	1:A:170:PHE:N	2.82	0.47
1:A:205:ASN:C	1:A:207:ASP:N	2.68	0.47
1:A:223:ILE:H	1:A:223:ILE:HD12	1.75	0.47
1:A:153:LYS:HE3	1:A:155:SER:HB2	1.96	0.47
1:A:223:ILE:CG2	1:A:224:LEU:N	2.77	0.47
1:B:342:LEU:HD22	1:B:345:ARG:HD3	1.96	0.47
1:A:115:LEU:HD22	1:A:119:ILE:CD1	2.44	0.47
1:A:139:ILE:H	1:A:139:ILE:HD13	1.79	0.47
1:B:238:ILE:HG13	1:B:266:TYR:CD2	2.49	0.47
1:A:230:TYR:CD2	1:A:231:ILE:N	2.82	0.47
1:A:208:LEU:O	1:A:211:VAL:HB	2.15	0.47
1:B:52:VAL:O	1:B:110:LEU:HD22	2.14	0.47
1:B:206:VAL:O	1:B:209:TRP:N	2.46	0.47
1:B:243:THR:HG22	1:B:244:PRO:N	2.30	0.47
1:A:63:ASN:H	1:A:66:HIS:HE2	1.60	0.47
1:A:189:ARG:NE	3:A:501:SO4:O1	2.42	0.47
1:A:353:LYS:O	1:A:356:ILE:HB	2.14	0.47
1:A:130:TYR:O	1:A:133:TYR:HB3	2.14	0.47
1:A:131:LEU:HD23	1:A:165:LEU:HD12	1.95	0.47
1:A:189:ARG:HH12	1:A:227:GLY:C	2.18	0.47
1:A:32:ILE:CG1	1:A:40:VAL:HG13	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:PRO:HD2	1:A:279:LEU:HD12	1.97	0.47
1:A:139:ILE:O	1:A:141:HIS:N	2.48	0.47
1:B:62:GLN:HG2	1:B:63:ASN:OD1	2.14	0.47
1:B:57:LEU:HD21	1:B:106:ILE:HG13	1.97	0.47
1:A:169:ASP:C	1:A:170:PHE:CD1	2.88	0.46
1:A:143:HIS:ND1	1:A:312:VAL:CG2	2.78	0.46
1:B:136:LEU:C	1:B:138:GLY:H	2.19	0.46
1:B:32:ILE:HG21	1:B:42:ALA:HB2	1.95	0.46
1:A:92:PHE:C	1:A:92:PHE:CD1	2.88	0.46
1:A:240:GLN:O	1:A:241:LEU:HD23	2.15	0.46
1:A:280:PHE:CE1	1:A:294:ALA:HB3	2.49	0.46
1:A:81:ASN:O	1:A:82:HIS:HB2	2.14	0.46
1:B:50:ARG:NH2	1:B:109:GLU:HB3	2.30	0.46
1:B:73:GLU:HG2	1:B:77:MET:CE	2.45	0.46
1:A:80:VAL:HG22	1:A:85:ILE:HG21	1.94	0.46
1:B:148:ILE:CD1	1:B:148:ILE:N	2.77	0.46
1:B:216:GLY:HA2	1:B:298:LEU:HD11	1.96	0.46
1:B:286:HIS:O	1:B:287:ASN:HB3	2.15	0.46
1:A:198:LEU:CD1	1:A:252:LEU:HD21	2.38	0.46
1:B:210:SER:O	1:B:213:CYS:HB2	2.16	0.46
1:A:148:ILE:CD1	1:A:175:THR:HA	2.44	0.46
1:A:114:ASN:ND2	1:A:116:CYS:HB3	2.30	0.46
1:B:220:CYS:C	1:B:222:LYS:H	2.19	0.46
1:B:115:LEU:HA	1:B:118:VAL:CG2	2.46	0.46
1:B:305:ASP:O	1:B:306:ALA:C	2.54	0.46
1:A:157:ILE:HA	1:A:157:ILE:HD13	1.68	0.46
1:A:90:ASN:HB3	1:A:107:VAL:HG21	1.96	0.46
1:A:242:GLY:N	1:A:268:GLY:CA	2.78	0.46
1:A:214:ILE:O	1:A:217:GLU:N	2.48	0.46
1:A:183:GLU:N	1:A:184:PRO:CD	2.79	0.46
1:B:71:TYR:OH	1:B:340:LYS:HD2	2.14	0.46
1:B:125:HIS:HD1	1:B:320:TYR:HE1	1.64	0.46
1:B:118:VAL:O	1:B:121:MET:HG2	2.16	0.46
1:A:205:ASN:O	1:A:208:LEU:N	2.46	0.46
1:B:115:LEU:HA	1:B:118:VAL:HG23	1.97	0.46
1:B:123:LEU:HD12	1:B:128:MET:H	1.80	0.46
1:A:238:ILE:HG13	1:A:239:GLU:N	2.30	0.46
1:B:31:PRO:HA	1:B:41:CYS:SG	2.56	0.46
1:A:294:ALA:O	1:A:297:LEU:HB3	2.15	0.46
1:A:342:LEU:O	1:A:343:ASP:HB2	2.14	0.46
1:A:197:ILE:HG22	1:A:198:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:HG13	1:B:207:ASP:N	2.31	0.46
1:A:283:ASP:O	1:A:285:GLU:N	2.49	0.46
1:B:186:VAL:CG1	1:B:187:VAL:H	2.17	0.45
1:B:189:ARG:O	1:B:191:TYR:N	2.48	0.45
1:A:180:PHE:CD1	1:A:181:MET:N	2.77	0.45
1:A:172:LEU:CD2	1:A:172:LEU:N	2.80	0.45
1:B:180:PHE:O	1:B:181:MET:C	2.55	0.45
1:A:230:TYR:HD2	1:A:231:ILE:H	1.60	0.45
1:A:168:LEU:N	1:A:168:LEU:CD2	2.79	0.45
1:B:271:PHE:CD2	1:B:274:LEU:HD12	2.52	0.45
1:B:26:TYR:O	1:B:27:GLN:C	2.55	0.45
1:B:83:LYS:O	1:B:84:ASN:ND2	2.47	0.45
1:A:91:VAL:CG2	1:A:363:LEU:HB2	2.47	0.45
1:B:142:LEU:C	1:B:144:SER:H	2.20	0.45
1:A:90:ASN:HB3	1:A:107:VAL:CG2	2.47	0.45
1:B:263:ARG:HA	1:B:263:ARG:HD2	1.69	0.45
1:A:298:LEU:O	1:A:300:LYS:N	2.49	0.45
1:A:225:PHE:O	1:A:233:GLN:NE2	2.36	0.45
1:A:43:ALA:HB3	1:A:54:ILE:CD1	2.47	0.45
1:A:54:ILE:HD12	1:A:54:ILE:N	2.31	0.45
1:B:357:TYR:C	1:B:359:GLU:N	2.69	0.45
1:A:25:ARG:HB2	1:A:47:ILE:HG22	1.98	0.45
1:B:195:GLU:HB3	1:B:200:MET:HE3	1.97	0.45
1:A:114:ASN:O	1:A:116:CYS:N	2.50	0.45
1:B:131:LEU:O	1:B:132:LEU:C	2.52	0.45
1:B:133:TYR:HB2	1:B:321:ILE:HG23	1.99	0.45
1:A:160:LYS:O	1:A:162:ASP:N	2.50	0.45
1:A:90:ASN:ND2	1:A:91:VAL:N	2.64	0.45
1:A:281:PRO:O	1:A:282:ALA:C	2.55	0.45
1:A:298:LEU:C	1:A:300:LYS:H	2.19	0.45
1:B:142:LEU:HG	1:B:147:ILE:HB	1.98	0.45
1:A:233:GLN:O	1:A:234:TRP:C	2.55	0.45
1:A:225:PHE:CZ	1:A:237:VAL:HG23	2.51	0.45
1:B:13:VAL:HG21	1:B:29:LEU:CD2	2.46	0.45
1:A:220:CYS:O	1:A:221:HIS:CB	2.65	0.45
1:A:133:TYR:O	1:A:136:LEU:HB2	2.16	0.45
1:A:325:TYR:CE1	1:A:330:ALA:HB1	2.53	0.44
1:B:89:LEU:HD11	1:B:109:GLU:HA	1.98	0.44
1:A:86:ILE:HD12	1:A:86:ILE:HA	1.74	0.44
1:B:230:TYR:CE2	1:B:231:ILE:HD11	2.52	0.44
1:B:214:ILE:O	1:B:215:MET:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:O	1:A:342:LEU:HD13	2.17	0.44
1:A:112:ASP:OD1	1:A:161:SER:HB2	2.17	0.44
1:A:165:LEU:HD23	1:A:165:LEU:C	2.37	0.44
1:A:80:VAL:HG22	1:A:81:ASN:H	1.83	0.44
1:B:228:ARG:O	1:B:229:ASP:CB	2.64	0.44
1:B:114:ASN:HD22	4:B:1001:73Q:H12	1.83	0.44
1:A:228:ARG:HG3	1:A:228:ARG:NH1	2.31	0.44
1:A:143:HIS:C	1:A:145:ALA:H	2.21	0.44
1:A:297:LEU:O	1:A:300:LYS:HB2	2.17	0.44
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.83	0.44
1:B:111:MET:HG3	1:B:158:VAL:HB	2.00	0.44
1:B:67:ALA:O	1:B:68:LYS:C	2.55	0.44
1:B:71:TYR:CE1	1:B:355:LEU:HB3	2.52	0.44
1:B:271:PHE:CZ	1:B:302:LEU:HD12	2.52	0.44
1:A:112:ASP:HB3	2:F:562:LEU:HD12	1.98	0.44
4:A:901:73Q:H31	4:A:901:73Q:O1	2.18	0.44
1:B:89:LEU:HG	1:B:109:GLU:N	2.33	0.44
1:A:29:LEU:HD23	1:A:29:LEU:C	2.38	0.44
1:A:311:SER:O	1:A:315:ALA:N	2.48	0.44
1:A:229:ASP:O	1:A:230:TYR:C	2.56	0.44
1:A:11:TYR:O	1:A:21:THR:HA	2.17	0.44
1:A:293:GLN:NE2	1:A:319:PRO:CB	2.81	0.44
1:B:284:SER:HB3	1:B:285:GLU:H	1.62	0.44
1:A:197:ILE:HD11	1:A:233:GLN:CG	2.47	0.44
1:B:198:LEU:HD13	1:B:252:LEU:CD2	2.47	0.44
1:B:339:ASP:O	1:B:341:GLN:N	2.51	0.44
1:B:117:GLN:NE2	2:G:562:LEU:HB3	2.32	0.44
1:A:119:ILE:HG22	1:A:120:GLN:N	2.32	0.44
1:B:90:ASN:HB3	1:B:107:VAL:HB	2.00	0.44
1:B:296:ASP:HB3	1:B:318:HIS:CE1	2.53	0.44
1:A:246:PRO:HA	1:A:249:MET:HB2	2.00	0.44
1:A:139:ILE:HG23	1:A:152:LEU:HD11	1.99	0.44
1:A:168:LEU:O	1:A:169:ASP:HB3	2.18	0.44
1:A:127:ARG:NH1	2:F:559:THR:O	2.51	0.44
1:B:32:ILE:HG13	1:B:41:CYS:HA	2.00	0.44
1:A:55:LYS:O	1:A:106:ILE:N	2.49	0.44
1:A:24:LYS:C	1:A:26:TYR:H	2.21	0.44
1:A:118:VAL:HA	1:A:121:MET:CG	2.45	0.43
1:B:90:ASN:ND2	1:B:91:VAL:N	2.62	0.43
1:B:148:ILE:CG1	1:B:204:GLU:HA	2.48	0.43
1:B:310:ILE:HD11	1:B:315:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HD12	1:B:128:MET:N	2.32	0.43
1:B:154:PRO:C	1:B:156:ASN:N	2.72	0.43
1:A:325:TYR:CE1	1:A:330:ALA:CB	3.01	0.43
1:B:167:ILE:O	1:B:168:LEU:HD22	2.18	0.43
1:A:243:THR:CG2	1:A:244:PRO:HD2	2.48	0.43
1:B:271:PHE:CE2	1:B:302:LEU:HD12	2.53	0.43
1:A:67:ALA:HB3	1:A:352:TRP:HD1	1.83	0.43
1:B:14:GLU:HG2	1:B:14:GLU:O	2.18	0.43
1:B:341:GLN:C	1:B:343:ASP:N	2.71	0.43
1:B:60:PRO:O	1:B:67:ALA:CB	2.64	0.43
1:A:68:LYS:HE2	1:A:72:ARG:NH2	2.34	0.43
1:B:99:GLU:O	1:B:99:GLU:HG2	2.18	0.43
1:A:111:MET:HG3	1:A:158:VAL:HG23	2.01	0.43
1:A:211:VAL:HA	1:A:214:ILE:HG13	1.99	0.43
1:B:348:THR:HG22	1:B:350:GLU:H	1.83	0.43
1:B:256:VAL:O	1:B:259:TYR:N	2.45	0.43
1:B:124:ASP:OD1	1:B:127:ARG:HD2	2.19	0.43
1:A:118:VAL:O	1:A:119:ILE:C	2.55	0.43
1:A:134:GLN:O	1:A:135:MET:C	2.55	0.43
1:A:293:GLN:NE2	1:A:319:PRO:HB2	2.33	0.43
1:A:82:HIS:HB3	1:A:85:ILE:HB	2.00	0.43
1:A:235:ASN:ND2	1:A:263:ARG:NH2	2.46	0.43
1:B:278:VAL:C	1:B:280:PHE:H	2.21	0.43
1:A:112:ASP:O	1:A:113:ALA:CB	2.66	0.43
1:A:49:GLU:O	1:A:50:ARG:CB	2.64	0.43
1:A:364:GLU:OE1	1:A:364:GLU:HA	2.18	0.43
1:A:114:ASN:O	1:A:117:GLN:N	2.51	0.43
1:B:57:LEU:HD21	1:B:106:ILE:CG1	2.49	0.43
1:B:276:PRO:O	1:B:278:VAL:N	2.44	0.43
1:A:225:PHE:CD1	1:A:237:VAL:HG23	2.53	0.43
1:B:329:GLU:OE1	2:G:556:ARG:NH2	2.50	0.43
1:B:193:ALA:HA	1:B:209:TRP:CD1	2.53	0.43
1:B:131:LEU:C	1:B:133:TYR:N	2.70	0.43
1:B:83:LYS:C	1:B:84:ASN:HD22	2.21	0.43
1:B:101:PHE:CD1	1:B:357:TYR:HD1	2.37	0.43
1:B:243:THR:HG22	1:B:244:PRO:CD	2.49	0.43
1:B:244:PRO:HB3	1:B:248:PHE:CD2	2.54	0.43
1:A:15:ILE:HD12	1:A:20:PHE:CE1	2.54	0.43
1:B:319:PRO:O	1:B:321:ILE:N	2.52	0.43
1:A:32:ILE:HG21	1:A:42:ALA:HB2	2.01	0.43
1:A:37:GLN:O	1:A:58:SER:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:GLN:HA	1:B:293:GLN:OE1	2.19	0.43
1:A:259:TYR:CE1	1:A:263:ARG:NE	2.87	0.43
1:B:130:TYR:O	1:B:134:GLN:HG3	2.19	0.43
1:A:244:PRO:CB	1:A:248:PHE:CD2	3.01	0.43
1:A:170:PHE:HD1	1:A:170:PHE:N	2.15	0.42
1:B:172:LEU:N	1:B:172:LEU:HD12	2.34	0.42
1:B:153:LYS:HE2	1:B:156:ASN:HD22	1.83	0.42
1:B:32:ILE:HG13	1:B:40:VAL:O	2.19	0.42
1:A:190:TYR:H	1:A:190:TYR:HD2	1.68	0.42
1:B:151:ASP:O	1:B:151:ASP:OD1	2.37	0.42
1:B:222:LYS:O	1:B:223:ILE:C	2.56	0.42
1:B:296:ASP:OD2	1:B:318:HIS:CE1	2.69	0.42
1:A:189:ARG:C	1:A:191:TYR:N	2.73	0.42
1:A:202:TYR:HD1	1:A:202:TYR:H	1.68	0.42
1:B:114:ASN:C	1:B:116:CYS:N	2.71	0.42
1:A:21:THR:HB	1:A:94:PRO:CB	2.49	0.42
1:A:127:ARG:O	1:A:128:MET:C	2.58	0.42
1:A:139:ILE:CD1	1:A:139:ILE:H	2.29	0.42
1:A:158:VAL:HG22	1:A:168:LEU:CD2	2.49	0.42
1:B:105:TYR:CD1	1:B:105:TYR:N	2.87	0.42
1:A:72:ARG:HH11	1:A:174:ARG:HG2	1.83	0.42
1:B:121:MET:HG3	1:B:123:LEU:HD23	2.01	0.42
1:B:123:LEU:HD22	1:B:123:LEU:HA	1.69	0.42
1:B:98:LEU:CD1	1:B:353:LYS:HG2	2.42	0.42
1:A:10:PHE:HD2	1:A:23:LEU:HD23	1.83	0.42
4:B:1001:73Q:H31	4:B:1001:73Q:HO1	1.85	0.42
1:B:323:VAL:CG2	1:B:324:TRP:H	2.32	0.42
1:B:338:PRO:O	1:B:339:ASP:HB3	2.19	0.42
1:A:301:MET:O	1:A:309:ARG:HD3	2.19	0.42
1:A:48:LEU:O	1:A:49:GLU:HB2	2.19	0.42
1:A:151:ASP:O	1:A:151:ASP:OD1	2.38	0.42
1:A:117:GLN:OE1	1:A:117:GLN:HA	2.19	0.42
1:A:298:LEU:C	1:A:300:LYS:N	2.73	0.42
1:B:92:PHE:CD1	1:B:92:PHE:C	2.93	0.42
1:B:215:MET:CE	1:B:298:LEU:HD13	2.50	0.42
1:A:53:ALA:HB2	1:A:110:LEU:HD12	2.01	0.42
1:A:321:ILE:O	1:A:322:ASN:C	2.57	0.42
1:B:149:HIS:O	1:B:150:ARG:CB	2.63	0.42
1:A:73:GLU:O	1:A:77:MET:HG2	2.20	0.42
1:A:85:ILE:HA	1:A:85:ILE:HD13	1.77	0.42
1:B:210:SER:O	1:B:213:CYS:N	2.39	0.42

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:CG2	1:B:42:ALA:H	2.32	0.42
1:B:235:ASN:HA	1:B:238:ILE:HG12	2.02	0.42
1:B:300:LYS:O	1:B:310:ILE:CG2	2.67	0.42
1:B:211:VAL:HG11	1:B:301:MET:HE2	2.02	0.42
1:A:28:ASN:OD1	1:A:44:TYR:HB3	2.20	0.42
1:A:139:ILE:HG22	1:A:143:HIS:NE2	2.35	0.42
1:B:136:LEU:C	1:B:138:GLY:N	2.73	0.42
1:B:315:ALA:C	1:B:317:GLN:N	2.73	0.42
1:A:356:ILE:O	1:A:359:GLU:HB2	2.20	0.42
1:A:214:ILE:O	1:A:215:MET:C	2.58	0.41
1:B:296:ASP:C	1:B:298:LEU:N	2.74	0.41
1:A:29:LEU:HD21	1:A:41:CYS:SG	2.60	0.41
1:A:182:MET:HG2	1:B:182:MET:SD	2.60	0.41
1:A:291:ALA:C	1:A:293:GLN:H	2.23	0.41
1:B:54:ILE:HA	1:B:106:ILE:O	2.19	0.41
1:A:101:PHE:CD2	1:A:357:TYR:CD1	3.08	0.41
1:A:61:PHE:CZ	1:A:102:GLN:HA	2.55	0.41
1:A:357:TYR:C	1:A:359:GLU:H	2.23	0.41
1:A:68:LYS:HE2	1:A:72:ARG:HH21	1.84	0.41
1:A:170:PHE:O	1:A:172:LEU:N	2.53	0.41
1:A:256:VAL:HG12	1:A:260:VAL:CG2	2.50	0.41
1:B:169:ASP:HB3	1:B:170:PHE:H	1.69	0.41
1:A:139:ILE:O	1:A:140:LYS:C	2.59	0.41
1:A:297:LEU:CB	1:A:318:HIS:HE1	2.27	0.41
1:B:111:MET:HG3	1:B:158:VAL:CG2	2.51	0.41
1:A:84:ASN:HA	1:A:165:LEU:O	2.20	0.41
1:B:195:GLU:HB3	1:B:200:MET:CE	2.50	0.41
1:A:134:GLN:OE1	1:A:165:LEU:N	2.49	0.41
1:B:297:LEU:O	1:B:301:MET:HB2	2.20	0.41
1:B:13:VAL:HG21	1:B:29:LEU:HD21	2.01	0.41
1:B:310:ILE:HG12	1:B:311:SER:O	2.21	0.41
1:A:102:GLN:O	1:A:103:ASP:CG	2.58	0.41
1:B:26:TYR:O	1:B:43:ALA:HB1	2.20	0.41
1:A:184:PRO:HB2	1:A:192:ARG:NH1	2.36	0.41
1:A:234:TRP:O	1:A:237:VAL:HG12	2.20	0.41
1:A:234:TRP:CD1	1:A:238:ILE:HD13	2.55	0.41
1:B:45:ASP:OD1	1:B:48:LEU:N	2.48	0.41
1:A:123:LEU:HD23	1:A:123:LEU:HA	1.81	0.41
1:A:71:TYR:CE1	1:A:355:LEU:HB3	2.56	0.41
1:A:197:ILE:HG22	1:A:198:LEU:N	2.34	0.41
1:A:53:ALA:HB3	1:A:108:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLY:CA	1:A:58:SER:H	2.28	0.41
1:A:223:ILE:HG22	1:A:224:LEU:H	1.85	0.41
1:B:60:PRO:HG2	1:B:61:PHE:H	1.86	0.41
1:B:190:TYR:HB2	1:B:191:TYR:CE1	2.55	0.41
1:B:136:LEU:HB3	1:B:316:LEU:HD12	1.98	0.41
1:B:297:LEU:HD13	1:B:318:HIS:CG	2.56	0.41
1:A:351:GLU:HG2	1:A:355:LEU:CD1	2.51	0.41
1:B:209:TRP:O	1:B:209:TRP:CD1	2.73	0.41
2:F:561:ASN:ND2	2:F:561:ASN:C	2.74	0.41
1:B:244:PRO:CB	1:B:248:PHE:CD2	3.04	0.41
1:A:212:GLY:O	1:A:214:ILE:N	2.54	0.40
1:A:139:ILE:CD1	1:A:167:ILE:HD11	2.47	0.40
1:A:280:PHE:HA	1:A:281:PRO:HD3	1.97	0.40
1:A:264:PRO:O	1:A:265:LYS:C	2.60	0.40
1:B:149:HIS:HE1	1:B:151:ASP:HB3	1.86	0.40
1:B:130:TYR:CZ	2:G:556:ARG:HD3	2.55	0.40
1:A:253:GLN:HB3	1:A:254:PRO:CD	2.43	0.40
1:A:245:CYS:HA	1:A:246:PRO:HD3	1.85	0.40
1:B:208:LEU:HA	1:B:208:LEU:HD22	1.82	0.40
1:A:224:LEU:HA	1:A:224:LEU:HD12	1.84	0.40
1:A:263:ARG:HA	1:A:264:PRO:HD3	1.93	0.40
1:B:84:ASN:OD1	1:B:137:CYS:SG	2.76	0.40
1:B:51:ASN:O	1:B:52:VAL:HG13	2.22	0.40
1:A:186:VAL:HG13	1:A:187:VAL:H	1.85	0.40
1:B:14:GLU:O	1:B:15:ILE:HD13	2.22	0.40
1:A:135:MET:HG2	1:A:139:ILE:HD11	2.02	0.40
1:A:137:CYS:O	1:A:140:LYS:HB3	2.21	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	354/370 (96%)	213 (60%)	92 (26%)	49 (14%)	0	4
1	B	355/370 (96%)	229 (64%)	81 (23%)	45 (13%)	0	6
2	F	8/11 (73%)	6 (75%)	1 (12%)	1 (12%)	0	6
2	G	8/11 (73%)	6 (75%)	2 (25%)	0	100	100
All	All	725/762 (95%)	454 (63%)	176 (24%)	95 (13%)	0	5

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	50	ARG
1	A	60	PRO
1	A	123	LEU
1	A	126	GLU
1	A	161	SER
1	A	181	MET
1	A	265	LYS
1	A	287	ASN
1	A	302	LEU
1	A	310	ILE
1	A	319	PRO
1	A	322	ASN
1	A	323	VAL
1	B	24	LYS
1	B	36	ALA
1	B	115	LEU
1	B	176	ALA
1	B	189	ARG
1	B	190	TYR
1	B	308	LYS
1	B	310	ILE
1	B	339	ASP
1	A	16	GLY
1	A	28	ASN
1	A	81	ASN
1	A	113	ALA
1	A	116	CYS
1	A	140	LYS
1	A	141	HIS
1	A	144	SER
1	A	163	CYS
1	A	188	THR

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Mol	Chain	Res	Type
1	A	203	LYS
1	A	204	GLU
1	A	292	SER
1	A	338	PRO
1	A	348	THR
1	A	364	GLU
1	B	18	SER
1	B	58	SER
1	B	62	GLN
1	B	74	LEU
1	B	83	LYS
1	B	86	ILE
1	B	126	GLU
1	B	155	SER
1	B	229	ASP
1	B	231	ILE
1	B	267	ALA
1	B	286	HIS
1	B	306	ALA
1	B	322	ASN
1	B	340	LYS
1	B	358	LYS
1	A	102	GLN
1	A	115	LEU
1	A	160	LYS
1	A	171	GLY
1	A	299	SER
2	F	561	ASN
1	B	25	ARG
1	B	49	GLU
1	B	101	PHE
1	B	125	HIS
1	B	186	VAL
1	B	235	ASN
1	B	264	PRO
1	B	336	LYS
1	A	25	ARG
1	A	174	ARG
1	A	176	ALA
1	A	229	ASP
1	A	339	ASP
1	B	78	LYS

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Mol	Chain	Res	Type
1	B	169	ASP
1	A	108	MET
1	A	169	ASP
1	A	315	ALA
1	B	64	GLN
1	B	67	ALA
1	B	91	VAL
1	B	277	ASP
1	B	316	LEU
1	A	235	ASN
1	A	284	SER
1	B	76	LEU
1	B	250	LYS
1	A	139	ILE
1	A	211	VAL
1	A	360	VAL
1	B	260	VAL
1	A	159	VAL
1	B	335	PRO
1	B	338	PRO

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	315/334 (94%)	274 (87%)	41 (13%)	5	27
1	B	314/334 (94%)	288 (92%)	26 (8%)	14	50
2	F	9/11 (82%)	7 (78%)	2 (22%)	1	6
2	G	9/11 (82%)	9 (100%)	0	100	100
All	All	647/690 (94%)	578 (89%)	69 (11%)	8	37

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	PHE

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Mol	Chain	Res	Type
1	A	51	ASN
1	A	61	PHE
1	A	66	HIS
1	A	69	ARG
1	A	73	GLU
1	A	86	ILE
1	A	95	GLN
1	A	101	PHE
1	A	115	LEU
1	A	118	VAL
1	A	119	ILE
1	A	124	ASP
1	A	139	ILE
1	A	148	ILE
1	A	150	ARG
1	A	157	ILE
1	A	168	LEU
1	A	172	LEU
1	A	174	ARG
1	A	180	PHE
1	A	188	THR
1	A	202	TYR
1	A	208	LEU
1	A	213	CYS
1	A	230	TYR
1	A	249	MET
1	A	258	THR
1	A	263	ARG
1	A	273	LYS
1	A	277	ASP
1	A	304	ILE
1	A	312	VAL
1	A	317	GLN
1	A	319	PRO
1	A	322	ASN
1	A	324	TRP
1	A	345	ARG
1	A	352	TRP
1	A	359	GLU
1	A	364	GLU
2	F	558	THR
2	F	561	ASN

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Mol	Chain	Res	Type
1	B	22	VAL
1	B	28	ASN
1	B	52	VAL
1	B	59	ARG
1	B	76	LEU
1	B	90	ASN
1	B	103	ASP
1	B	104	VAL
1	B	123	LEU
1	B	156	ASN
1	B	174	ARG
1	B	180	PHE
1	B	197	ILE
1	B	208	LEU
1	B	230	TYR
1	B	263	ARG
1	B	264	PRO
1	B	271	PHE
1	B	272	GLU
1	B	285	GLU
1	B	286	HIS
1	B	304	ILE
1	B	313	ASP
1	B	324	TRP
1	B	352	TRP
1	B	362	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	37	GLN
1	A	84	ASN
1	A	90	ASN
1	A	120	GLN
1	A	235	ASN
1	A	317	GLN
1	A	322	ASN
2	F	561	ASN
1	B	28	ASN
1	B	37	GLN
1	B	90	ASN

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Mol	Chain	Res	Type
1	B	102	GLN
1	B	117	GLN
1	B	141	HIS
1	B	233	GLN
1	B	318	HIS
1	B	347	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 ligands 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	$\#|Z| > 2$
3	SO4	A	501	-	4,4,4	1.33	0	6,6,6	0.06	0
3	SO4	A	601	-	4,4,4	0.96	0	6,6,6	0.13	0
4	73Q	A	901	-	15,20,20	2.27	3 (20%)	15,31,31	2.87	8 (53%)
4	73Q	B	1001	-	15,20,20	1.93	4 (26%)	15,31,31	2.77	7 (46%)
3	SO4	B	701	-	4,4,4	1.29	0	6,6,6	0.10	0
3	SO4	B	801	-	4,4,4	1.09	0	6,6,6	0.09	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
3	SO4	A	501	-	-	0/0/0/0	0/0/0/0
3	SO4	A	601	-	-	0/0/0/0	0/0/0/0
4	73Q	A	901	-	-	0/0/0/0	0/3/3/3
4	73Q	B	1001	-	-	0/0/0/0	0/3/3/3
3	SO4	B	701	-	-	0/0/0/0	0/0/0/0
3	SO4	B	801	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1001	73Q	C8-CL	-2.51	1.68	1.74
4	B	1001	73Q	C11-C10	2.31	1.44	1.41
4	B	1001	73Q	C7-C8	3.04	1.43	1.38
4	A	901	73Q	C11-C10	3.20	1.45	1.41
4	A	901	73Q	C7-C8	3.32	1.44	1.38
4	B	1001	73Q	C10-C5	4.38	1.44	1.41
4	A	901	73Q	C10-C5	5.82	1.45	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	73Q	C6-C5-C10	-3.57	114.94	119.97
4	B	1001	73Q	C6-C5-C10	-3.37	115.21	119.97
4	A	901	73Q	C7-C8-C9	-2.86	118.14	121.87
4	B	1001	73Q	C7-C8-C9	-2.36	118.79	121.87
4	A	901	73Q	C7-C8-CL	2.05	122.71	119.35
4	B	1001	73Q	C1-C2-N1	2.38	125.07	119.73
4	A	901	73Q	C1-C2-N1	2.53	125.39	119.73
4	B	1001	73Q	C7-C6-C5	2.81	124.21	119.42
4	A	901	73Q	C7-C6-C5	3.01	124.55	119.42
4	B	1001	73Q	C3-N2-N1	3.61	124.06	118.05
4	A	901	73Q	C3-N2-N1	3.88	124.50	118.05
4	A	901	73Q	C2-N1-N2	5.14	108.91	104.34
4	B	1001	73Q	C2-N1-N2	5.27	109.03	104.34
4	B	1001	73Q	C6-C5-N3	6.06	125.92	119.76
4	A	901	73Q	C6-C5-N3	6.16	126.03	119.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	SO4	3	0
4	A	901	73Q	5	0
4	B	1001	73Q	4	0
3	B	701	SO4	1	0

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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.