Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 03:00 PM EDT

PDB ID	:	1T8Y
Title	:	Crystal Structure of E.coli AMP Nucleosidase complexed with phosphate
Authors	:	Zhang, Y.; Cottet, S.E.; Ealick, S.E.
Deposited on	:	2004-05-13
Resolution	:	3.00 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:

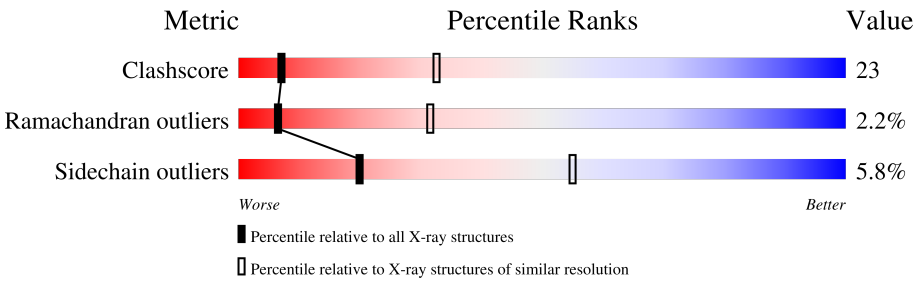
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	484	61% 31% • 5%
1	B	484	60% 31% • 5%
1	C	484	61% 31% • 5%
1	D	484	58% 33% • 5%
1	E	484	57% 35% • 5%
1	F	484	57% 34% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22005 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 AMP nucleosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	461	3648	2317	641	681	5	4	0	0	0
1	B	461	3648	2317	641	681	5	4	0	0	0
1	C	461	3648	2317	641	681	5	4	0	0	0
1	D	461	3648	2317	641	681	5	4	0	0	0
1	E	461	3648	2317	641	681	5	4	0	0	0
1	F	461	3648	2317	641	681	5	4	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MSE	MET	MODIFIED RESIDUE	UNP P15272
A	260	MSE	MET	MODIFIED RESIDUE	UNP P15272
A	302	MSE	MET	MODIFIED RESIDUE	UNP P15272
A	404	MSE	MET	MODIFIED RESIDUE	UNP P15272
B	138	MSE	MET	MODIFIED RESIDUE	UNP P15272
B	260	MSE	MET	MODIFIED RESIDUE	UNP P15272
B	302	MSE	MET	MODIFIED RESIDUE	UNP P15272
B	404	MSE	MET	MODIFIED RESIDUE	UNP P15272
C	138	MSE	MET	MODIFIED RESIDUE	UNP P15272
C	260	MSE	MET	MODIFIED RESIDUE	UNP P15272
C	302	MSE	MET	MODIFIED RESIDUE	UNP P15272
C	404	MSE	MET	MODIFIED RESIDUE	UNP P15272
D	138	MSE	MET	MODIFIED RESIDUE	UNP P15272
D	260	MSE	MET	MODIFIED RESIDUE	UNP P15272
D	302	MSE	MET	MODIFIED RESIDUE	UNP P15272
D	404	MSE	MET	MODIFIED RESIDUE	UNP P15272
E	138	MSE	MET	MODIFIED RESIDUE	UNP P15272

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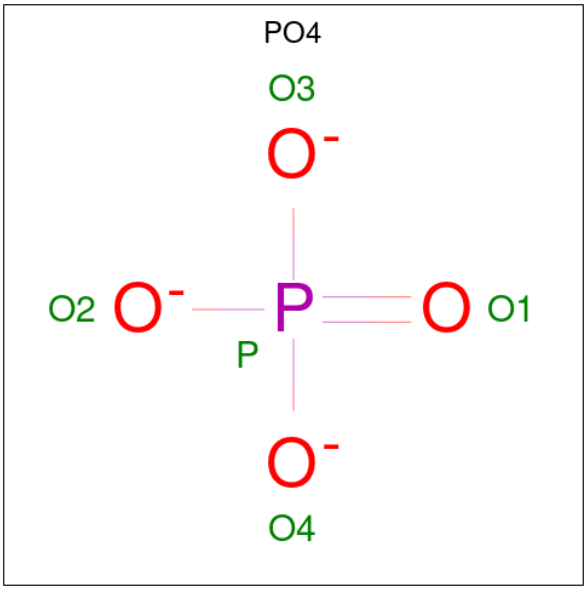
Chain	Residue	Modelled	Actual	Comment	Reference
E	260	MSE	MET	MODIFIED RESIDUE	UNP P15272
E	302	MSE	MET	MODIFIED RESIDUE	UNP P15272
E	404	MSE	MET	MODIFIED RESIDUE	UNP P15272
F	138	MSE	MET	MODIFIED RESIDUE	UNP P15272
F	260	MSE	MET	MODIFIED RESIDUE	UNP P15272
F	302	MSE	MET	MODIFIED RESIDUE	UNP P15272
F	404	MSE	MET	MODIFIED RESIDUE	UNP P15272

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0
2	D	1	5	4	1	0	0
2	E	1	5	4	1	0	0
2	F	1	5	4	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	15	15	15	0	0
			Total	O		
3	B	21	21	21	0	0
			Total	O		
3	C	12	12	12	0	0
			Total	O		
3	D	13	13	13	0	0
			Total	O		
3	E	14	14	14	0	0
			Total	O		
3	F	12	12	12	0	0

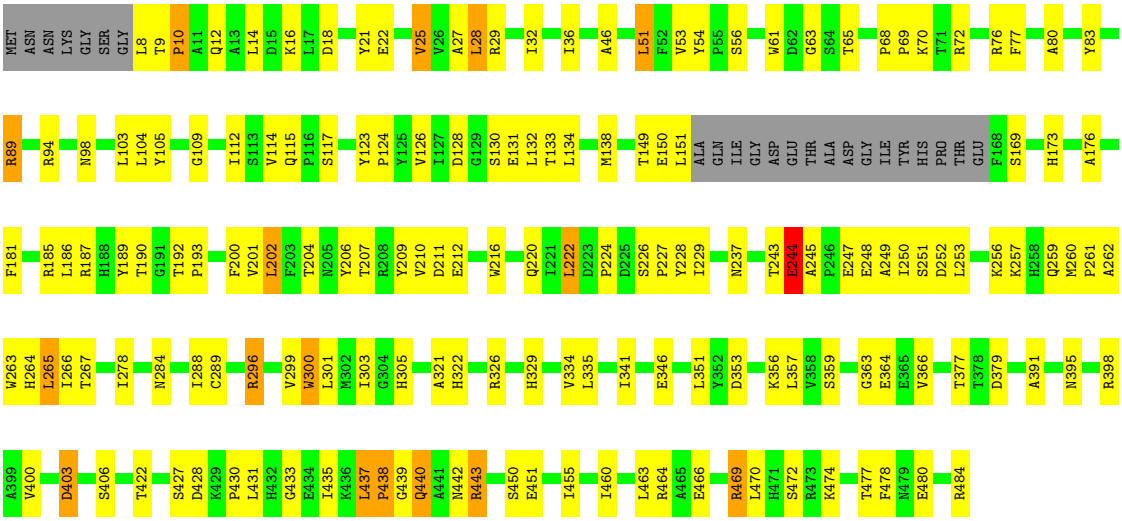
3 Residue-property plots (i)

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. 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. 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.

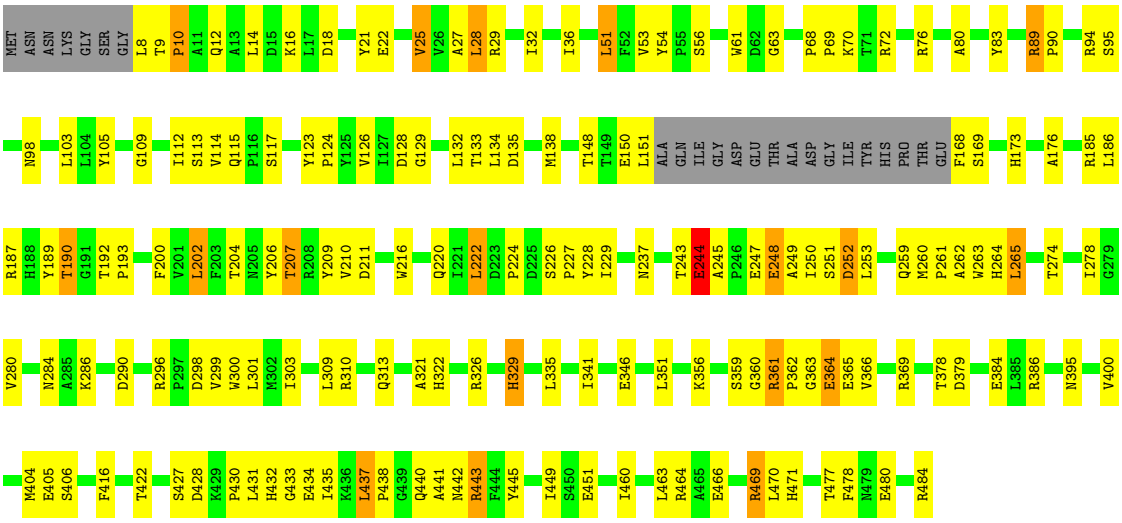
• Molecule 1: AMP nucleosidase

Chain A:



• Molecule 1: AMP nucleosidase

Chain B:



• Molecule 1: AMP nucleosidase

Chain C: 61% 31% • 5%

MET ASN ASN LYS GLY SER GLY L8 T9 P10 A11 Q12 A13 L14 D15 K16 L17 D18 Y21 E22 V25 V26 A27 L28 I32 I36 A46 L51 F52 V53 Y54 P55 S56 W61 D62 G63 P68 P69 K70 T71 R72 R76 F77 T78 H79 A80 Y83 R89

R94 N98 L101 T102 L103 L104 Y105 G109 I112 S113 V114 S117 Y123 V126 I127 D128 G129 S130 E131 L132 T133 L134 D135 R136 S137 M138 L151 ALA GLN ILE GLY ASP GLU THR ALA ASP GLY ILE TYR HIS PRO THR GLU F168 H173 R177 F181 R185

L186 R187 T190 G191 T192 P193 F200 V201 L202 F203 T204 N205 Y206 T207 R208 Y209 V210 D211 E212 W216 Q220 I221 L222 D223 P224 D225 S226 P227 Y228 I229 N237 T243 E244 A245 P246 E247 E248 A249 I250 S251 D252 L253 K257 H258 Q259 M260 P261 A262 W263 H264 L265 I278

G279 V280 N284 H291 V294 L295 R296 P297 D298 V299 W300 L301 M302 I303 R310 Q313 H322 A323 Y324 L325 R326 D327 D328 H329 V330 L335 I341 P342 E346 V347 L351 K356 S359 G360 R361 P362 G363 E364 D379 E384 L385 R386 Y387 N395 L396

V400 E405 S406 S427 D428 L431 H432 G433 E434 I435 K436 L437 P438 A441 N442 R443 F444 Y445 E446 S450 E451 I455 I460 L463 R464 A465 E466 R469 L470 H471 S472 R473 K474 T477 F478 N479 E480 R484

• Molecule 1: AMP nucleosidase

Chain D: 58% 33% • 5%

MET ASN ASN LYS GLY SER GLY L8 T9 P10 A11 Q12 A13 L14 D18 Y21 E22 V25 V26 A27 L28 I32 I36 A46 L51 F52 V53 Y54 P55 S56 W61 D62 G63 S64 T65 P68 P69 R72 R76 F77 A80 Y83 R89 R94 S95

Y96 L97 N98 E99 Q100 L103 L104 Y105 G109 I112 S113 V114 Q115 P116 S117 I121 P122 Y123 P124 Y125 V126 I127 D128 G129 S130 E131 L132 T133 L134 M138 T148 T149 E150 L151 ALA GLN ILE GLY ASP GLU THR ALA ASP GLY ILE TYR HIS PRO THR GLU F168 S169 H173

A176 S182 R185 L186 R187 H188 Y189 T190 G191 T192 P193 F200 V201 L202 F203 T204 N205 Y206 T207 R208 Y209 V210 D211 W216 Q220 I221 L222 D223 P224 D225 S226 P227 Y228 I229 N237 E242 T243 E244 A245 P246 E247 E248 A249 I250 S251 D252 Q259 M260 P261 A262 W263

H264 L265 I266 T267 T274 I278 N284 H291 R296 P297 D298 V299 W300 L301 M302 I303 G304 H305 R310 Q313 A321 H322 L325 R326 H329 V330 L335 P336 P337 I341 E346 V347 L351 K356 S359 G360 R361 P362 G363 E364 E365 V366 R369

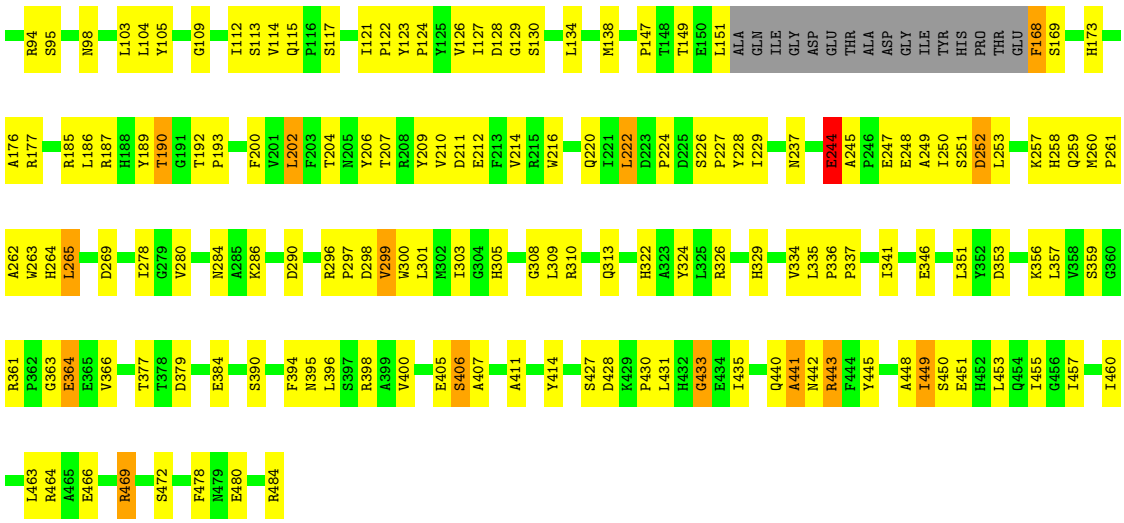
T377 T378 D379 D380 R381 A391 N395 V400 D403 S406 T422 S427 D428 K429 P430 L431 E434 I435 K436 L437 Q440 A441 N442 R443 F444 Y445 I449 S450 E451 I455 I460 L463 R464 A465 E466 R469 L470 H471 S472 R473 K474 T477 F478 N479

E480 F483 R484

• Molecule 1: AMP nucleosidase

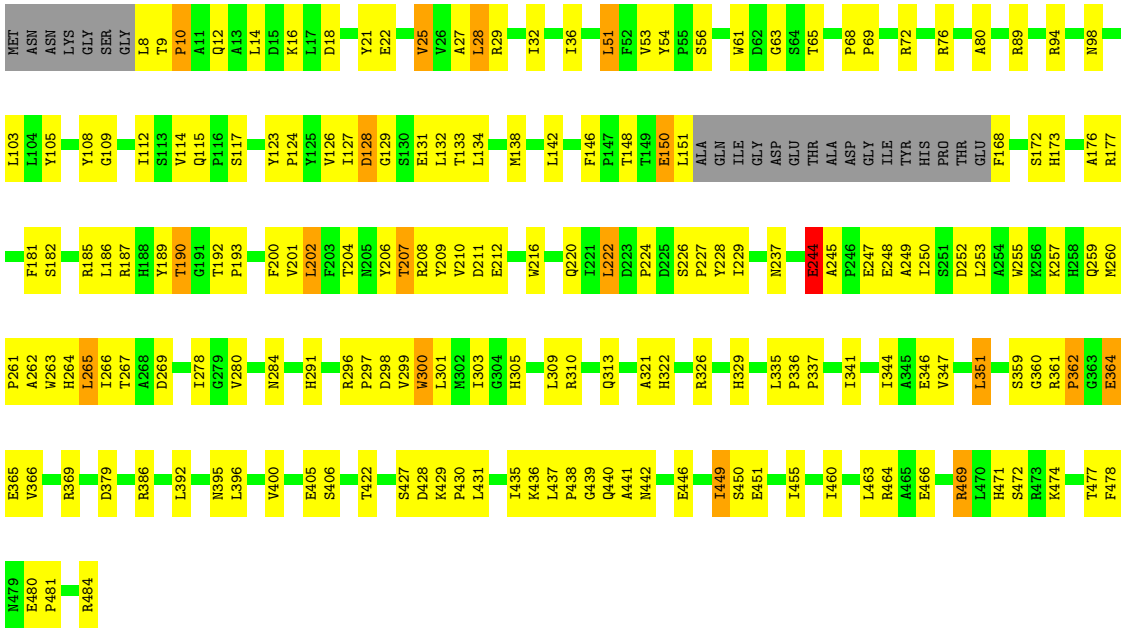
Chain E: 57% 35% • 5%

MET ASN ASN LYS GLY SER GLY L8 T9 P10 A11 Q12 A13 L14 D15 K16 L17 D18 Y21 E22 V25 V26 A27 L28 R29 I32 I36 L51 F52 V53 Y54 P55 S56 G63 S64 T65 P68 P69 K70 T71 R72 R76 F77 A80 G81 S82 Y83 R89 P90 T91



- Molecule 1: AMP nucleosidase

Chain F:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	268.50Å 268.50Å 114.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.07 – 3.00	Depositor
% Data completeness (in resolution range)	96.0 (34.07-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22005	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

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: PO4

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	0.43	0/3738	0.64	0/5088
1	B	0.44	0/3738	0.64	0/5088
1	C	0.44	0/3738	0.66	0/5088
1	D	0.44	0/3738	0.64	0/5088
1	E	0.46	0/3738	0.64	0/5088
1	F	0.44	0/3738	0.65	0/5088
All	All	0.44	0/22428	0.64	0/30528

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	3648	0	3576	171	0
1	B	3648	0	3576	177	0
1	C	3648	0	3576	176	0
1	D	3648	0	3576	176	0
1	E	3648	0	3576	178	0
1	F	3648	0	3576	199	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
3	A	15	0	0	1	0
3	B	21	0	0	1	0
3	C	12	0	0	2	0
3	D	13	0	0	1	0
3	E	14	0	0	1	0
3	F	12	0	0	1	0
All	All	22005	0	21456	987	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 23.

All (987) 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:B:443:ARG:HH11	1:B:443:ARG:HB3	1.20	1.05
1:E:192:THR:HG21	1:E:264:HIS:NE2	1.72	1.05
1:C:192:THR:HG21	1:C:264:HIS:NE2	1.75	1.02
1:A:131:GLU:HB2	1:B:441:ALA:HB3	1.41	1.02
1:C:151:LEU:H	1:C:151:LEU:HD22	1.22	1.02
1:A:192:THR:HG21	1:A:264:HIS:NE2	1.75	1.01
1:F:192:THR:HG21	1:F:264:HIS:NE2	1.76	1.00
1:B:192:THR:HG21	1:B:264:HIS:NE2	1.77	0.99
1:E:36:ILE:HA	1:E:138:MSE:HE1	1.40	0.99
1:E:190:THR:CG2	1:E:192:THR:HB	1.93	0.98
1:C:190:THR:CG2	1:C:192:THR:HB	1.95	0.96
1:D:190:THR:CG2	1:D:192:THR:HB	1.95	0.96
1:A:190:THR:CG2	1:A:192:THR:HB	1.99	0.92
1:C:18:ASP:O	1:C:22:GLU:HG2	1.70	0.92
1:D:469:ARG:HH21	1:E:364:GLU:HB3	1.35	0.90
1:F:190:THR:CG2	1:F:192:THR:HB	2.01	0.90
1:D:192:THR:HG21	1:D:264:HIS:NE2	1.86	0.90
1:F:192:THR:HG21	1:F:264:HIS:HE2	1.35	0.90
1:B:190:THR:CG2	1:B:192:THR:HB	2.01	0.89
1:A:202:LEU:HD13	1:A:460:ILE:HD11	1.55	0.89
1:F:18:ASP:O	1:F:22:GLU:HG2	1.72	0.89
1:A:36:ILE:HA	1:A:138:MSE:HE1	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:THR:HG22	1:A:192:THR:HB	1.55	0.88
1:E:18:ASP:O	1:E:22:GLU:HG2	1.74	0.87
1:F:202:LEU:HD13	1:F:460:ILE:HD11	1.53	0.87
1:C:36:ILE:HA	1:C:138:MSE:HE1	1.54	0.87
1:C:190:THR:HG22	1:C:192:THR:HB	1.56	0.87
1:E:361:ARG:NH1	1:E:361:ARG:HB2	1.90	0.85
1:E:441:ALA:HB3	1:F:131:GLU:HB2	1.59	0.84
1:E:186:LEU:O	1:E:190:THR:HB	1.77	0.84
1:E:202:LEU:HD13	1:E:460:ILE:HD11	1.58	0.84
1:B:186:LEU:O	1:B:190:THR:HB	1.78	0.84
1:A:435:ILE:HG21	1:B:185:ARG:HH22	1.40	0.84
1:A:18:ASP:O	1:A:22:GLU:HG2	1.79	0.83
1:C:384:GLU:HB3	1:D:151:LEU:HD21	1.61	0.82
1:B:18:ASP:O	1:B:22:GLU:HG2	1.78	0.82
1:B:469:ARG:HH21	1:C:364:GLU:HB3	1.44	0.82
1:E:190:THR:HG22	1:E:192:THR:HB	1.61	0.82
1:D:395:ASN:HD22	1:E:478:PHE:HD1	1.29	0.81
1:A:186:LEU:O	1:A:190:THR:HB	1.80	0.81
1:B:36:ILE:HA	1:B:138:MSE:HE1	1.63	0.81
1:D:18:ASP:O	1:D:22:GLU:HG2	1.79	0.81
1:D:190:THR:HG22	1:D:192:THR:HB	1.61	0.80
1:F:36:ILE:HA	1:F:138:MSE:HE1	1.64	0.80
1:C:186:LEU:O	1:C:190:THR:HB	1.82	0.80
1:A:437:LEU:HD13	1:A:440:GLN:OE1	1.83	0.79
1:B:202:LEU:HD13	1:B:460:ILE:HD11	1.63	0.79
1:F:134:LEU:HD23	1:F:138:MSE:HB3	1.65	0.78
1:B:72:ARG:NH1	1:B:103:LEU:HD22	1.98	0.78
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.49	0.78
1:C:72:ARG:NH1	1:C:103:LEU:HD22	1.99	0.78
1:B:190:THR:HG22	1:B:192:THR:HB	1.65	0.78
1:F:32:ILE:HD11	1:F:123:TYR:HB2	1.66	0.77
1:B:443:ARG:HH11	1:B:443:ARG:CB	1.95	0.77
1:D:395:ASN:HD21	1:E:478:PHE:H	1.32	0.77
1:A:185:ARG:HH22	1:B:435:ILE:HG21	1.48	0.77
1:B:469:ARG:NH2	1:C:364:GLU:HB3	2.00	0.77
1:F:127:ILE:HD13	1:F:132:LEU:HG	1.67	0.76
1:D:72:ARG:NH1	1:D:103:LEU:HD22	2.01	0.76
1:D:186:LEU:O	1:D:190:THR:HB	1.84	0.76
1:D:207:THR:O	1:D:210:VAL:HG22	1.86	0.76
1:C:32:ILE:HD11	1:C:123:TYR:HB2	1.67	0.76
1:F:440:GLN:HG2	1:F:441:ALA:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:436:LYS:HG3	1:F:442:ASN:HD22	1.49	0.76
1:F:430:PRO:HA	1:F:435:ILE:HG12	1.66	0.76
1:E:441:ALA:CB	1:F:131:GLU:HB2	2.15	0.76
1:B:469:ARG:HH11	1:B:469:ARG:HG2	1.51	0.75
1:A:132:LEU:HB3	1:A:134:LEU:HD13	1.68	0.75
1:B:395:ASN:ND2	1:C:478:PHE:H	1.85	0.75
1:E:134:LEU:HD23	1:E:138:MSE:HB3	1.68	0.75
1:A:469:ARG:HG2	1:A:469:ARG:HH11	1.52	0.75
1:A:443:ARG:HH21	1:B:135:ASP:HA	1.53	0.74
1:F:190:THR:HG22	1:F:192:THR:HB	1.68	0.74
1:F:192:THR:HG21	1:F:264:HIS:CD2	2.23	0.74
1:D:395:ASN:ND2	1:E:478:PHE:H	1.86	0.73
1:F:186:LEU:O	1:F:190:THR:HB	1.87	0.73
1:B:395:ASN:HD21	1:C:478:PHE:H	1.34	0.72
1:B:478:PHE:H	1:C:395:ASN:HD21	1.37	0.72
1:D:134:LEU:HD23	1:D:138:MSE:HB3	1.71	0.72
1:A:437:LEU:HD12	1:A:437:LEU:H	1.55	0.72
1:D:202:LEU:HD13	1:D:460:ILE:HD11	1.69	0.72
1:A:472:SER:OG	1:A:474:LYS:HG3	1.89	0.72
1:B:478:PHE:H	1:C:395:ASN:ND2	1.88	0.72
1:B:469:ARG:HH21	1:C:364:GLU:CB	2.01	0.72
1:B:134:LEU:HD23	1:B:138:MSE:HB3	1.72	0.71
1:E:228:TYR:CG	1:E:265:LEU:HD13	2.25	0.71
1:A:32:ILE:HD11	1:A:123:TYR:HB2	1.69	0.71
1:D:326:ARG:HG2	1:D:326:ARG:HH11	1.56	0.71
1:E:72:ARG:NH1	1:E:103:LEU:HD22	2.06	0.71
1:A:395:ASN:HD22	1:F:478:PHE:HD1	1.38	0.71
1:C:437:LEU:HD23	1:D:188:HIS:CD2	2.26	0.71
1:B:192:THR:HG21	1:B:264:HIS:CD2	2.25	0.70
1:D:437:LEU:HD13	1:D:440:GLN:HG3	1.72	0.70
1:F:207:THR:O	1:F:210:VAL:HG22	1.92	0.70
1:E:361:ARG:HB2	1:E:361:ARG:HH11	1.57	0.69
1:D:127:ILE:HD13	1:D:132:LEU:HG	1.74	0.69
1:E:469:ARG:HG2	1:E:469:ARG:HH11	1.56	0.69
1:A:134:LEU:HD23	1:A:138:MSE:HB3	1.75	0.69
1:E:27:ALA:HB1	1:E:51:LEU:CD2	2.22	0.69
1:B:32:ILE:HD11	1:B:123:TYR:HB2	1.74	0.69
1:D:364:GLU:HB3	1:E:469:ARG:HH21	1.58	0.68
1:C:202:LEU:HD13	1:C:460:ILE:HD11	1.75	0.68
1:E:63:GLY:HA3	1:E:80:ALA:HB2	1.75	0.68
1:E:192:THR:HG21	1:E:264:HIS:CD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:THR:HG21	1:C:264:HIS:CD2	2.28	0.68
1:D:192:THR:HG21	1:D:264:HIS:CD2	2.28	0.68
1:C:36:ILE:HA	1:C:138:MSE:CE	2.23	0.68
1:B:259:GLN:O	1:B:260:MSE:HG3	1.94	0.68
1:E:207:THR:O	1:E:210:VAL:HG22	1.94	0.68
1:B:478:PHE:HD1	1:C:395:ASN:HD22	1.41	0.68
1:A:190:THR:HG23	1:A:262:ALA:HB3	1.74	0.67
1:C:134:LEU:HD23	1:C:138:MSE:HB3	1.75	0.67
1:A:477:THR:HB	1:F:395:ASN:HD21	1.58	0.67
1:D:436:LYS:HG3	1:D:442:ASN:ND2	2.09	0.67
1:E:228:TYR:CD1	1:E:265:LEU:HD13	2.29	0.67
1:A:259:GLN:O	1:A:260:MSE:HG3	1.94	0.67
1:C:469:ARG:HG2	1:C:469:ARG:HH11	1.60	0.67
1:D:63:GLY:HA3	1:D:80:ALA:HB2	1.77	0.67
1:F:9:THR:HG23	1:F:12:GLN:NE2	2.10	0.67
1:C:228:TYR:CG	1:C:265:LEU:HD13	2.30	0.66
1:C:259:GLN:O	1:C:260:MSE:HG3	1.93	0.66
1:F:220:GLN:O	1:F:226:SER:HB3	1.95	0.66
1:C:187:ARG:HH11	1:C:187:ARG:HG3	1.60	0.66
1:B:27:ALA:HB1	1:B:51:LEU:CD2	2.25	0.66
1:A:395:ASN:HD21	1:F:478:PHE:H	1.42	0.66
1:D:469:ARG:HG2	1:D:469:ARG:HH11	1.61	0.66
1:A:395:ASN:ND2	1:F:478:PHE:H	1.94	0.66
1:B:329:HIS:HD2	1:B:379:ASP:OD2	1.79	0.66
1:B:395:ASN:HD22	1:C:478:PHE:HD1	1.43	0.65
1:A:359:SER:HA	1:A:451:GLU:OE1	1.97	0.65
1:C:27:ALA:HB1	1:C:51:LEU:CD2	2.25	0.65
1:D:478:PHE:H	1:E:395:ASN:HD21	1.43	0.65
1:A:27:ALA:HB1	1:A:51:LEU:CD2	2.25	0.65
1:B:443:ARG:HB3	1:B:443:ARG:NH1	2.04	0.65
1:F:151:LEU:HD22	1:F:151:LEU:H	1.62	0.65
1:D:259:GLN:O	1:D:260:MSE:HG3	1.97	0.65
1:D:478:PHE:HD1	1:E:395:ASN:HD22	1.46	0.64
1:E:440:GLN:O	1:E:442:ASN:N	2.28	0.64
1:D:36:ILE:HA	1:D:138:MSE:HE1	1.78	0.64
1:D:83:TYR:HA	1:D:169:SER:O	1.98	0.64
1:B:326:ARG:HG2	1:B:326:ARG:HH11	1.63	0.64
1:C:260:MSE:HG2	1:C:278:ILE:HA	1.79	0.64
1:E:190:THR:HG23	1:E:262:ALA:HB3	1.79	0.64
1:C:190:THR:HG23	1:C:262:ALA:HB3	1.80	0.64
1:F:132:LEU:HB3	1:F:134:LEU:HD13	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:440:GLN:HG2	1:F:441:ALA:N	2.13	0.64
1:E:36:ILE:HA	1:E:138:MSE:CE	2.21	0.64
1:C:151:LEU:HD22	1:C:151:LEU:N	2.05	0.63
1:F:326:ARG:HG2	1:F:326:ARG:HH11	1.63	0.63
1:E:185:ARG:HH22	1:F:435:ILE:HG22	1.62	0.63
1:A:105:TYR:O	1:A:109:GLY:HA2	1.98	0.63
1:B:364:GLU:HB3	1:C:469:ARG:HH21	1.64	0.63
1:D:360:GLY:O	1:D:362:PRO:HD3	1.99	0.63
1:E:222:LEU:O	1:E:224:PRO:HD3	1.97	0.63
1:E:228:TYR:HB3	1:E:265:LEU:HD22	1.80	0.63
1:E:326:ARG:HH11	1:E:326:ARG:HG2	1.64	0.63
1:F:27:ALA:HB1	1:F:51:LEU:CD2	2.28	0.63
1:F:63:GLY:HA3	1:F:80:ALA:HB2	1.80	0.63
1:C:63:GLY:HA3	1:C:80:ALA:HB2	1.80	0.63
1:B:469:ARG:HH21	1:C:364:GLU:CG	2.10	0.63
1:D:227:PRO:O	1:D:229:ILE:HG23	1.99	0.63
1:D:364:GLU:HB3	1:E:469:ARG:NH2	2.14	0.63
1:A:63:GLY:HA3	1:A:80:ALA:HB2	1.81	0.62
1:A:192:THR:HG21	1:A:264:HIS:CD2	2.34	0.62
1:E:463:LEU:O	1:E:466:GLU:HB2	2.00	0.62
1:B:190:THR:HG23	1:B:262:ALA:HB3	1.81	0.62
1:B:28:LEU:HD13	1:B:126:VAL:HG21	1.81	0.62
1:D:8:LEU:HB3	1:D:112:ILE:O	2.00	0.62
1:D:228:TYR:HB3	1:D:265:LEU:HD22	1.80	0.62
1:F:296:ARG:HD3	1:F:484:ARG:OXT	2.00	0.62
1:B:63:GLY:HA3	1:B:80:ALA:HB2	1.82	0.62
1:B:361:ARG:HG2	1:B:365:GLU:CD	2.19	0.62
1:B:469:ARG:HG2	1:B:469:ARG:NH1	2.13	0.62
1:B:310:ARG:H	1:B:313:GLN:NE2	1.98	0.62
1:E:237:ASN:HD21	1:E:248:GLU:HB2	1.65	0.62
1:A:8:LEU:HD12	1:A:9:THR:H	1.64	0.62
1:B:228:TYR:CG	1:B:265:LEU:HD13	2.34	0.62
1:B:286:LYS:NZ	1:B:290:ASP:OD1	2.32	0.62
1:D:469:ARG:NH2	1:E:364:GLU:HB3	2.12	0.62
1:F:228:TYR:CG	1:F:265:LEU:HD13	2.35	0.62
1:A:77:PHE:CE2	1:A:104:LEU:HD22	2.34	0.62
1:D:132:LEU:HB3	1:D:134:LEU:HD13	1.82	0.62
1:F:463:LEU:O	1:F:466:GLU:HB2	1.99	0.61
1:B:361:ARG:HH11	1:B:361:ARG:HB2	1.64	0.61
1:E:8:LEU:HD12	1:E:9:THR:H	1.64	0.61
1:C:151:LEU:H	1:C:151:LEU:CD2	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:THR:HB	1:D:10:PRO:HD2	1.82	0.61
1:E:253:LEU:HD13	1:F:252:ASP:OD1	2.01	0.61
1:D:478:PHE:H	1:E:395:ASN:ND2	1.98	0.61
1:A:469:ARG:HG2	1:A:469:ARG:NH1	2.14	0.61
1:C:326:ARG:HH11	1:C:326:ARG:HG2	1.65	0.61
1:D:190:THR:HG21	1:D:192:THR:HB	1.83	0.61
1:E:190:THR:HG21	1:E:192:THR:HB	1.82	0.61
1:A:21:TYR:O	1:A:25:VAL:HG12	2.01	0.61
1:B:363:GLY:O	1:B:366:VAL:HG22	2.01	0.60
1:E:27:ALA:HB1	1:E:51:LEU:HD21	1.82	0.60
1:B:245:ALA:HB1	1:B:247:GLU:OE1	2.01	0.60
1:E:185:ARG:NH2	1:F:435:ILE:HG22	2.16	0.60
1:A:185:ARG:NH2	1:B:435:ILE:HG21	2.16	0.60
1:A:478:PHE:H	1:F:395:ASN:ND2	1.99	0.60
1:A:53:VAL:HG13	1:A:117:SER:OG	2.01	0.60
1:B:105:TYR:O	1:B:109:GLY:HA2	2.01	0.60
1:D:32:ILE:HD11	1:D:123:TYR:HB2	1.83	0.60
1:E:259:GLN:O	1:E:260:MSE:HG3	2.01	0.60
1:E:356:LYS:HE2	1:E:363:GLY:H	1.67	0.60
1:E:9:THR:HB	1:E:10:PRO:HD2	1.82	0.60
1:C:216:TRP:O	1:C:220:GLN:HG2	2.00	0.60
1:F:206:TYR:HB3	1:F:209:TYR:CD2	2.36	0.60
1:F:259:GLN:O	1:F:260:MSE:HG3	2.01	0.60
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.65	0.60
1:D:364:GLU:H	1:D:364:GLU:CD	2.05	0.60
1:E:14:LEU:HD13	1:E:94:ARG:HD3	1.83	0.60
1:E:220:GLN:O	1:E:226:SER:HB3	2.02	0.60
1:A:437:LEU:O	1:A:439:GLY:N	2.34	0.59
1:D:27:ALA:HB1	1:D:51:LEU:CD2	2.32	0.59
1:D:335:LEU:HD21	1:D:341:ILE:HD11	1.84	0.59
1:E:173:HIS:HE1	1:E:480:GLU:OE2	1.85	0.59
1:F:216:TRP:O	1:F:220:GLN:HG2	2.03	0.59
1:F:253:LEU:HD21	1:F:257:LYS:NZ	2.16	0.59
1:A:220:GLN:O	1:A:226:SER:HB3	2.02	0.59
1:A:228:TYR:CG	1:A:265:LEU:HD13	2.37	0.59
1:D:21:TYR:O	1:D:25:VAL:HG12	2.02	0.59
1:D:105:TYR:O	1:D:109:GLY:HA2	2.01	0.59
1:A:435:ILE:HG21	1:B:185:ARG:NH2	2.13	0.59
1:F:228:TYR:HB3	1:F:265:LEU:HD22	1.84	0.59
1:A:56:SER:HB2	1:A:117:SER:HB3	1.85	0.59
1:A:204:THR:HG22	1:A:303:ILE:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:THR:HG23	1:D:193:PRO:HD2	1.85	0.59
1:D:329:HIS:HD2	1:D:379:ASP:OD2	1.85	0.59
1:C:9:THR:HG22	1:C:105:TYR:OH	2.02	0.59
1:E:21:TYR:O	1:E:25:VAL:HG12	2.03	0.59
1:B:132:LEU:HB3	1:B:134:LEU:CD1	2.33	0.58
1:F:173:HIS:HE1	1:F:480:GLU:OE2	1.84	0.58
1:A:72:ARG:NH1	1:A:103:LEU:HD22	2.19	0.58
1:C:329:HIS:HD2	1:C:379:ASP:OD2	1.86	0.58
1:F:335:LEU:HD21	1:F:341:ILE:HD11	1.86	0.58
1:A:329:HIS:HD2	1:A:379:ASP:OD2	1.87	0.58
1:A:335:LEU:HD21	1:A:341:ILE:HD11	1.84	0.58
1:B:134:LEU:HB3	1:B:138:MSE:HB3	1.85	0.58
1:D:437:LEU:HD12	1:D:437:LEU:H	1.67	0.58
1:E:8:LEU:HD12	1:E:9:THR:N	2.19	0.58
1:A:440:GLN:HE21	1:A:440:GLN:HA	1.69	0.58
1:D:190:THR:HG23	1:D:262:ALA:HB3	1.85	0.58
1:D:244:GLU:HG2	1:D:245:ALA:H	1.69	0.58
1:A:443:ARG:HD3	1:B:133:THR:CG2	2.34	0.58
1:C:220:GLN:O	1:C:226:SER:HB3	2.03	0.58
1:C:463:LEU:O	1:C:466:GLU:HB2	2.03	0.58
1:A:244:GLU:CD	1:A:244:GLU:N	2.57	0.58
1:B:200:PHE:CZ	1:B:464:ARG:HG3	2.39	0.58
1:D:14:LEU:HD11	1:D:98:ASN:HB2	1.86	0.58
1:E:384:GLU:HB3	1:F:151:LEU:HG	1.85	0.58
1:A:463:LEU:HD22	1:A:470:LEU:HD13	1.86	0.58
1:B:469:ARG:NH2	1:C:364:GLU:OE1	2.37	0.58
1:E:14:LEU:HD11	1:E:98:ASN:HB2	1.86	0.58
1:E:244:GLU:HG2	1:E:245:ALA:H	1.69	0.58
1:E:359:SER:HA	1:E:451:GLU:OE1	2.03	0.58
1:B:220:GLN:O	1:B:226:SER:HB3	2.04	0.58
1:B:227:PRO:O	1:B:229:ILE:HG23	2.03	0.58
1:C:244:GLU:CD	1:C:244:GLU:N	2.57	0.58
1:A:53:VAL:HG12	1:A:54:TYR:O	2.04	0.57
1:D:364:GLU:OE1	1:E:469:ARG:NH2	2.37	0.57
1:E:296:ARG:HD3	1:E:484:ARG:OXT	2.04	0.57
1:A:132:LEU:HB3	1:A:134:LEU:CD1	2.33	0.57
1:A:326:ARG:HG2	1:A:326:ARG:NH1	2.19	0.57
1:F:208:ARG:HD3	1:F:446:GLU:OE1	2.04	0.57
1:A:151:LEU:HD21	1:B:435:ILE:HD11	1.86	0.57
1:C:435:ILE:HG21	1:D:185:ARG:HH22	1.68	0.57
1:C:359:SER:HA	1:C:451:GLU:OE1	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:280:VAL:HA	1:F:405:GLU:OE2	2.05	0.57
1:F:469:ARG:HG2	1:F:469:ARG:HH11	1.70	0.57
1:A:200:PHE:CZ	1:A:464:ARG:HG3	2.39	0.57
1:A:466:GLU:O	1:A:469:ARG:HB2	2.05	0.57
1:C:173:HIS:HE1	1:C:480:GLU:OE2	1.87	0.57
1:E:244:GLU:OE2	1:E:244:GLU:N	2.38	0.57
1:B:237:ASN:HD21	1:B:248:GLU:HB2	1.70	0.57
1:F:346:GLU:H	1:F:346:GLU:CD	2.07	0.57
1:C:9:THR:HB	1:C:10:PRO:HD2	1.85	0.56
1:C:228:TYR:HB3	1:C:265:LEU:HD22	1.87	0.56
1:E:91:THR:HB	3:E:515:HOH:O	2.06	0.56
1:F:361:ARG:HB3	1:F:365:GLU:CD	2.26	0.56
1:A:8:LEU:HD12	1:A:9:THR:N	2.20	0.56
1:B:9:THR:HB	1:B:10:PRO:HD2	1.88	0.56
1:D:216:TRP:O	1:D:220:GLN:HG2	2.05	0.56
1:E:9:THR:HG22	1:E:105:TYR:OH	2.04	0.56
1:B:442:ASN:ND2	1:B:445:TYR:CB	2.69	0.56
1:A:245:ALA:HB1	1:A:247:GLU:OE1	2.05	0.56
1:B:437:LEU:HD12	1:B:440:GLN:OE1	2.06	0.56
1:C:237:ASN:HD21	1:C:248:GLU:HB2	1.70	0.56
1:D:310:ARG:H	1:D:313:GLN:NE2	2.03	0.56
1:E:250:ILE:HG22	1:E:250:ILE:O	2.04	0.56
1:A:207:THR:O	1:A:210:VAL:HG22	2.05	0.56
1:A:227:PRO:O	1:A:229:ILE:HG23	2.06	0.56
1:A:463:LEU:O	1:A:466:GLU:HB2	2.06	0.56
1:C:207:THR:O	1:C:210:VAL:HG22	2.05	0.56
1:C:469:ARG:HG2	1:C:469:ARG:NH1	2.20	0.56
1:D:134:LEU:HB3	1:D:138:MSE:CB	2.36	0.56
1:F:105:TYR:O	1:F:109:GLY:HA2	2.06	0.56
1:F:202:LEU:HD13	1:F:460:ILE:CD1	2.33	0.56
1:F:244:GLU:N	1:F:244:GLU:OE2	2.38	0.56
1:B:16:LYS:HD3	1:B:114:VAL:HB	1.87	0.56
1:C:442:ASN:ND2	1:C:445:TYR:CB	2.68	0.56
1:C:442:ASN:ND2	1:C:445:TYR:HB3	2.20	0.56
1:C:435:ILE:HG21	1:D:185:ARG:NH2	2.21	0.56
1:E:261:PRO:HB2	1:E:263:TRP:CZ3	2.41	0.56
1:A:9:THR:HG23	1:A:12:GLN:NE2	2.21	0.55
1:A:356:LYS:HE2	1:A:363:GLY:O	2.07	0.55
1:C:228:TYR:CD1	1:C:265:LEU:HD13	2.41	0.55
1:E:227:PRO:O	1:E:229:ILE:HG23	2.05	0.55
1:A:437:LEU:HD12	1:A:437:LEU:N	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:THR:O	1:B:210:VAL:HG22	2.07	0.55
1:D:9:THR:HG23	1:D:12:GLN:NE2	2.21	0.55
1:E:9:THR:HG23	1:E:12:GLN:NE2	2.21	0.55
1:E:469:ARG:HG2	1:E:469:ARG:NH1	2.18	0.55
1:A:36:ILE:HA	1:A:138:MSE:CE	2.31	0.55
1:A:133:THR:HB	1:B:443:ARG:HD3	1.88	0.55
1:A:435:ILE:CG2	1:B:185:ARG:HH22	2.17	0.55
1:C:200:PHE:CZ	1:C:464:ARG:HG3	2.42	0.55
1:F:436:LYS:HG3	1:F:442:ASN:ND2	2.18	0.55
1:B:8:LEU:HD12	1:B:9:THR:H	1.70	0.55
1:B:151:LEU:N	1:B:151:LEU:HD22	2.22	0.55
1:E:310:ARG:H	1:E:313:GLN:NE2	2.03	0.55
1:F:134:LEU:HB3	1:F:138:MSE:CB	2.36	0.55
1:C:310:ARG:H	1:C:313:GLN:NE2	2.04	0.55
1:C:364:GLU:N	1:C:364:GLU:CD	2.60	0.55
1:D:326:ARG:HG2	1:D:326:ARG:NH1	2.22	0.55
1:E:28:LEU:HD13	1:E:126:VAL:HG21	1.88	0.55
1:F:54:TYR:CD2	1:F:176:ALA:HB1	2.41	0.55
1:C:364:GLU:CD	1:C:364:GLU:H	2.10	0.55
1:E:129:GLY:O	1:E:130:SER:HB3	2.06	0.55
1:C:261:PRO:HB2	1:C:263:TRP:CZ3	2.42	0.55
1:D:189:TYR:HB3	1:D:260:MSE:HE3	1.88	0.55
1:D:466:GLU:O	1:D:469:ARG:HB2	2.07	0.55
1:E:151:LEU:N	1:E:151:LEU:HD22	2.22	0.55
1:F:222:LEU:O	1:F:224:PRO:HD3	2.06	0.55
1:A:27:ALA:HB1	1:A:51:LEU:HD21	1.87	0.55
1:A:261:PRO:HB2	1:A:263:TRP:CZ3	2.42	0.55
1:D:469:ARG:HG2	1:D:469:ARG:NH1	2.22	0.55
1:F:329:HIS:HD2	1:F:379:ASP:OD2	1.90	0.55
1:B:14:LEU:HD13	1:B:94:ARG:HD3	1.90	0.54
1:D:364:GLU:CG	1:E:469:ARG:HH21	2.20	0.54
1:A:8:LEU:HB3	1:A:112:ILE:O	2.07	0.54
1:C:105:TYR:O	1:C:109:GLY:HA2	2.07	0.54
1:D:187:ARG:HG3	1:D:187:ARG:HH11	1.70	0.54
1:E:253:LEU:HD21	1:E:257:LYS:NZ	2.23	0.54
1:B:216:TRP:O	1:B:220:GLN:HG2	2.07	0.54
1:B:228:TYR:HB3	1:B:265:LEU:HD22	1.88	0.54
1:B:430:PRO:HA	1:B:435:ILE:HG12	1.89	0.54
1:E:187:ARG:HG3	1:E:187:ARG:HH11	1.73	0.54
1:E:190:THR:HG22	1:E:192:THR:N	2.23	0.54
1:A:346:GLU:H	1:A:346:GLU:CD	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:SER:HB2	1:C:117:SER:HB3	1.90	0.54
1:C:227:PRO:O	1:C:229:ILE:HG23	2.06	0.54
1:D:8:LEU:HD12	1:D:9:THR:H	1.73	0.54
1:D:28:LEU:HD13	1:D:126:VAL:HG21	1.90	0.54
1:E:53:VAL:HG13	1:E:117:SER:OG	2.06	0.54
1:E:252:ASP:OD1	1:F:253:LEU:HD13	2.07	0.54
1:F:190:THR:HG23	1:F:262:ALA:HB3	1.90	0.54
1:A:190:THR:HG21	1:A:192:THR:HB	1.86	0.54
1:B:8:LEU:HB3	1:B:112:ILE:O	2.07	0.54
1:D:128:ASP:O	1:D:129:GLY:O	2.26	0.54
1:E:335:LEU:HD21	1:E:341:ILE:HD11	1.89	0.54
1:F:8:LEU:HD12	1:F:9:THR:H	1.72	0.54
1:F:261:PRO:HB2	1:F:263:TRP:CZ3	2.43	0.54
1:F:369:ARG:HG2	1:F:369:ARG:HH11	1.71	0.54
1:C:27:ALA:HB1	1:C:51:LEU:HD21	1.90	0.54
1:D:220:GLN:O	1:D:226:SER:HB3	2.07	0.54
1:A:65:THR:HG23	3:A:521:HOH:O	2.06	0.54
1:A:237:ASN:HD21	1:A:248:GLU:HB2	1.72	0.54
1:A:260:MSE:HG2	1:A:278:ILE:HA	1.89	0.54
1:C:151:LEU:HD21	1:D:430:PRO:O	2.06	0.54
1:E:466:GLU:O	1:E:469:ARG:HB2	2.08	0.54
1:C:14:LEU:HD11	1:C:98:ASN:HB2	1.90	0.54
1:D:222:LEU:O	1:D:224:PRO:HD3	2.08	0.54
1:E:216:TRP:O	1:E:220:GLN:HG2	2.07	0.54
1:F:244:GLU:HG2	1:F:245:ALA:H	1.73	0.54
1:D:192:THR:HG23	1:D:193:PRO:CD	2.38	0.54
1:D:364:GLU:CB	1:E:469:ARG:HH21	2.21	0.54
1:E:237:ASN:ND2	1:E:248:GLU:HB2	2.23	0.54
1:B:21:TYR:O	1:B:25:VAL:HG12	2.08	0.54
1:B:395:ASN:HD21	1:C:477:THR:HB	1.73	0.53
1:D:200:PHE:CZ	1:D:464:ARG:HG3	2.42	0.53
1:F:9:THR:HB	1:F:10:PRO:HD2	1.89	0.53
1:E:200:PHE:CZ	1:E:464:ARG:HG3	2.43	0.53
1:B:261:PRO:HB2	1:B:263:TRP:CZ3	2.43	0.53
1:C:132:LEU:HD13	1:C:134:LEU:CD1	2.37	0.53
1:B:206:TYR:HB3	1:B:209:TYR:CD2	2.43	0.53
1:E:9:THR:OG1	1:E:12:GLN:HG3	2.09	0.53
1:F:310:ARG:H	1:F:313:GLN:NE2	2.06	0.53
1:F:437:LEU:HD13	1:F:440:GLN:OE1	2.09	0.53
1:A:430:PRO:HA	1:A:435:ILE:HG12	1.91	0.53
1:E:8:LEU:HB3	1:E:112:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:ARG:HG3	1:F:187:ARG:HH11	1.73	0.53
1:F:361:ARG:HB2	1:F:361:ARG:NH1	2.24	0.53
1:B:134:LEU:HB3	1:B:138:MSE:CB	2.38	0.53
1:B:442:ASN:ND2	1:B:445:TYR:HB3	2.23	0.53
1:C:8:LEU:HD12	1:C:9:THR:H	1.73	0.53
1:E:105:TYR:O	1:E:109:GLY:HA2	2.08	0.53
1:B:296:ARG:NH2	1:B:416:PHE:O	2.36	0.53
1:D:8:LEU:HD12	1:D:9:THR:N	2.23	0.53
1:D:244:GLU:N	1:D:244:GLU:OE2	2.42	0.53
1:F:253:LEU:HD11	1:F:257:LYS:HE3	1.90	0.53
1:F:436:LYS:CG	1:F:442:ASN:HD22	2.20	0.53
1:B:244:GLU:N	1:B:244:GLU:CD	2.61	0.53
1:D:260:MSE:HG2	1:D:278:ILE:HA	1.91	0.53
1:E:151:LEU:HD22	1:E:151:LEU:H	1.74	0.53
1:F:206:TYR:HB3	1:F:209:TYR:HD2	1.71	0.53
1:A:185:ARG:CZ	1:B:437:LEU:HD21	2.39	0.53
1:B:9:THR:HG23	1:B:12:GLN:NE2	2.23	0.53
1:C:190:THR:HG21	1:C:192:THR:HB	1.87	0.53
1:C:21:TYR:O	1:C:25:VAL:HG12	2.09	0.52
1:C:247:GLU:C	1:C:249:ALA:H	2.12	0.52
1:B:228:TYR:CD1	1:B:265:LEU:HD13	2.44	0.52
1:F:245:ALA:HB1	1:F:247:GLU:OE1	2.10	0.52
1:B:187:ARG:HG3	1:B:187:ARG:HH11	1.74	0.52
1:F:8:LEU:HD12	1:F:9:THR:N	2.24	0.52
1:F:27:ALA:HB1	1:F:51:LEU:HD21	1.92	0.52
1:D:9:THR:HG22	1:D:105:TYR:OH	2.09	0.52
1:C:296:ARG:HD3	1:C:484:ARG:OXT	2.08	0.52
1:C:384:GLU:HB3	1:D:151:LEU:CD2	2.36	0.52
1:D:56:SER:HB2	1:D:117:SER:HB3	1.92	0.52
1:E:435:ILE:HG21	1:F:185:ARG:HH22	1.75	0.52
1:F:440:GLN:CG	1:F:441:ALA:H	2.20	0.52
1:A:14:LEU:HD11	1:A:98:ASN:HB2	1.92	0.52
1:A:151:LEU:HD23	1:B:430:PRO:O	2.09	0.52
1:D:204:THR:HG22	1:D:303:ILE:O	2.10	0.52
1:D:463:LEU:O	1:D:466:GLU:HB2	2.10	0.52
1:A:9:THR:HB	1:A:10:PRO:HD2	1.91	0.52
1:A:296:ARG:HD3	1:A:484:ARG:OXT	2.09	0.52
1:B:250:ILE:HG22	1:B:250:ILE:O	2.10	0.52
1:D:435:ILE:HG22	1:D:435:ILE:O	2.10	0.52
1:F:227:PRO:O	1:F:229:ILE:HG23	2.09	0.52
1:C:132:LEU:HD12	1:C:132:LEU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:TYR:HB3	1:E:209:TYR:CD2	2.45	0.52
1:E:309:LEU:N	1:E:313:GLN:HE22	2.08	0.52
1:F:21:TYR:O	1:F:25:VAL:HG12	2.10	0.52
1:F:53:VAL:HG13	1:F:117:SER:OG	2.10	0.52
1:F:228:TYR:CD1	1:F:265:LEU:HD13	2.45	0.52
1:F:237:ASN:HD21	1:F:248:GLU:HB2	1.73	0.52
1:A:206:TYR:HB3	1:A:209:TYR:CD2	2.45	0.52
1:C:53:VAL:HG13	1:C:117:SER:OG	2.10	0.52
1:F:72:ARG:NH1	1:F:103:LEU:HD22	2.24	0.52
1:A:451:GLU:O	1:A:455:ILE:HG13	2.09	0.52
1:E:363:GLY:O	1:E:366:VAL:HG22	2.10	0.52
1:F:16:LYS:HD3	1:F:114:VAL:HB	1.91	0.52
1:B:134:LEU:HD23	1:B:138:MSE:HE3	1.91	0.51
1:C:72:ARG:HH12	1:C:103:LEU:HD22	1.75	0.51
1:E:472:SER:HB2	2:E:504:PO4:O1	2.10	0.51
1:B:132:LEU:HB3	1:B:134:LEU:HD13	1.92	0.51
1:D:427:SER:O	1:D:428:ASP:HB3	2.10	0.51
1:F:177:ARG:HG3	1:F:177:ARG:HH11	1.74	0.51
1:A:123:TYR:CG	1:A:124:PRO:HD3	2.46	0.51
1:B:260:MSE:HG2	1:B:278:ILE:HA	1.92	0.51
1:C:472:SER:OG	1:C:474:LYS:HG3	2.11	0.51
1:A:53:VAL:HG13	1:A:117:SER:HG	1.75	0.51
1:A:321:ALA:HB3	1:A:422:THR:HB	1.92	0.51
1:E:127:ILE:HG22	1:E:130:SER:H	1.76	0.51
1:A:32:ILE:O	1:A:36:ILE:HG13	2.09	0.51
1:B:14:LEU:HD11	1:B:98:ASN:HB2	1.93	0.51
1:C:245:ALA:HB1	1:C:247:GLU:OE1	2.10	0.51
1:D:190:THR:HG22	1:D:192:THR:N	2.25	0.51
1:D:210:VAL:HG23	1:D:211:ASP:N	2.24	0.51
1:F:296:ARG:NH1	1:F:484:ARG:O	2.43	0.51
1:A:185:ARG:HH22	1:B:435:ILE:CG2	2.19	0.51
1:F:36:ILE:HA	1:F:138:MSE:CE	2.38	0.51
1:D:9:THR:HB	1:D:10:PRO:CD	2.40	0.51
1:E:53:VAL:HG11	1:E:117:SER:O	2.11	0.51
1:B:222:LEU:O	1:B:224:PRO:HD3	2.11	0.51
1:D:247:GLU:C	1:D:249:ALA:H	2.13	0.51
1:C:253:LEU:HD21	1:C:257:LYS:NZ	2.25	0.51
1:E:9:THR:HB	1:E:10:PRO:CD	2.40	0.51
1:E:260:MSE:HG2	1:E:278:ILE:HA	1.93	0.51
1:A:478:PHE:HD1	1:F:395:ASN:HD22	1.59	0.51
1:B:280:VAL:HA	1:B:405:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:HIS:O	1:C:294:VAL:HG22	2.11	0.51
1:A:14:LEU:HD13	1:A:94:ARG:HD3	1.93	0.50
1:B:206:TYR:HB3	1:B:209:TYR:HD2	1.77	0.50
1:F:192:THR:HG23	1:F:193:PRO:HD2	1.93	0.50
1:B:298:ASP:OD1	1:B:471:HIS:HE1	1.95	0.50
1:C:8:LEU:HB3	1:C:112:ILE:O	2.11	0.50
1:C:132:LEU:HD12	1:C:132:LEU:N	2.26	0.50
1:D:321:ALA:HB3	1:D:422:THR:HB	1.94	0.50
1:B:466:GLU:O	1:B:469:ARG:HB2	2.12	0.50
1:C:222:LEU:O	1:C:224:PRO:HD3	2.12	0.50
1:E:185:ARG:HH22	1:F:435:ILE:CG2	2.25	0.50
1:A:149:THR:O	1:A:150:GLU:OE2	2.30	0.50
1:A:151:LEU:HG	1:B:384:GLU:HB3	1.93	0.50
1:B:72:ARG:HH12	1:B:103:LEU:HD22	1.72	0.50
1:B:237:ASN:ND2	1:B:248:GLU:HB2	2.26	0.50
1:B:247:GLU:C	1:B:249:ALA:H	2.14	0.50
1:D:250:ILE:O	1:D:250:ILE:HG22	2.11	0.50
1:E:253:LEU:HD11	1:E:257:LYS:HE3	1.94	0.50
1:F:54:TYR:CE2	1:F:176:ALA:HB1	2.46	0.50
1:F:260:MSE:HG2	1:F:278:ILE:HA	1.93	0.50
1:A:477:THR:HB	1:F:395:ASN:ND2	2.25	0.50
1:D:27:ALA:HB1	1:D:51:LEU:HD21	1.92	0.50
1:F:8:LEU:CD1	1:F:12:GLN:HB2	2.42	0.50
1:B:8:LEU:HD12	1:B:9:THR:N	2.26	0.50
1:B:427:SER:O	1:B:428:ASP:HB3	2.12	0.50
1:C:61:TRP:CE3	1:C:63:GLY:HA2	2.47	0.50
1:C:127:ILE:HG22	1:C:129:GLY:O	2.11	0.50
1:C:466:GLU:O	1:C:469:ARG:HB2	2.12	0.50
1:D:14:LEU:HD13	1:D:94:ARG:HD3	1.93	0.50
1:E:173:HIS:CE1	1:E:480:GLU:OE2	2.64	0.50
1:F:28:LEU:HD13	1:F:126:VAL:HG21	1.93	0.50
1:F:200:PHE:CZ	1:F:464:ARG:HG3	2.47	0.50
1:E:32:ILE:HD11	1:E:123:TYR:HB2	1.92	0.50
1:F:134:LEU:HB3	1:F:138:MSE:HB3	1.93	0.50
1:B:359:SER:HA	1:B:451:GLU:OE1	2.12	0.50
1:C:190:THR:HG22	1:C:192:THR:N	2.27	0.50
1:E:54:TYR:CD2	1:E:176:ALA:HB1	2.47	0.50
1:F:9:THR:HG22	1:F:105:TYR:OH	2.12	0.50
1:C:250:ILE:HG22	1:C:250:ILE:O	2.12	0.50
1:D:248:GLU:H	1:D:248:GLU:CD	2.14	0.50
1:E:326:ARG:NH2	1:E:335:LEU:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ILE:O	1:F:250:ILE:HG22	2.12	0.50
1:A:29:ARG:HH21	1:A:128:ASP:HB2	1.77	0.49
1:A:222:LEU:O	1:A:224:PRO:HD3	2.12	0.49
1:C:212:GLU:HG2	1:C:450:SER:HA	1.94	0.49
1:E:82:SER:O	1:E:168:PHE:N	2.45	0.49
1:D:237:ASN:HD21	1:D:248:GLU:HB2	1.76	0.49
1:E:329:HIS:HD2	1:E:379:ASP:OD2	1.94	0.49
1:F:451:GLU:O	1:F:455:ILE:HG13	2.12	0.49
1:C:69:PRO:O	1:C:76:ARG:HD2	2.12	0.49
1:C:296:ARG:NH1	1:C:484:ARG:O	2.44	0.49
1:A:173:HIS:HE1	1:A:480:GLU:OE2	1.95	0.49
1:D:472:SER:OG	1:D:474:LYS:HG3	2.13	0.49
1:E:206:TYR:HB3	1:E:209:TYR:HD2	1.77	0.49
1:E:245:ALA:HB1	1:E:247:GLU:OE1	2.12	0.49
1:F:173:HIS:CE1	1:F:480:GLU:OE2	2.65	0.49
1:F:210:VAL:HG23	1:F:211:ASP:N	2.27	0.49
1:A:250:ILE:O	1:A:250:ILE:HG22	2.13	0.49
1:C:192:THR:HG23	1:C:193:PRO:HD2	1.94	0.49
1:D:228:TYR:CG	1:D:265:LEU:HD13	2.48	0.49
1:A:478:PHE:H	1:F:395:ASN:HD21	1.60	0.49
1:B:204:THR:HG22	1:B:303:ILE:O	2.13	0.49
1:E:56:SER:HB3	1:E:115:GLN:O	2.12	0.49
1:F:8:LEU:HB3	1:F:112:ILE:O	2.12	0.49
1:F:359:SER:HA	1:F:451:GLU:OE1	2.12	0.49
1:C:53:VAL:HG11	1:C:117:SER:O	2.12	0.49
1:A:8:LEU:CD1	1:A:12:GLN:HB2	2.43	0.49
1:B:360:GLY:O	1:B:362:PRO:HD3	2.12	0.49
1:D:53:VAL:HG12	1:D:54:TYR:O	2.13	0.49
1:E:122:PRO:HA	1:E:147:PRO:O	2.13	0.49
1:A:253:LEU:HD21	1:A:257:LYS:NZ	2.28	0.49
1:C:53:VAL:HG11	1:C:117:SER:N	2.28	0.49
1:B:361:ARG:HB2	1:B:361:ARG:NH1	2.28	0.48
1:C:361:ARG:N	1:C:362:PRO:HD3	2.28	0.48
1:A:216:TRP:O	1:A:220:GLN:HG2	2.13	0.48
1:B:134:LEU:CD2	1:B:138:MSE:HE3	2.43	0.48
1:B:309:LEU:N	1:B:313:GLN:HE22	2.10	0.48
1:B:335:LEU:HD21	1:B:341:ILE:HD11	1.93	0.48
1:C:127:ILE:HG22	1:C:127:ILE:O	2.13	0.48
1:F:56:SER:HB3	1:F:115:GLN:O	2.13	0.48
1:F:364:GLU:CD	1:F:364:GLU:H	2.16	0.48
1:A:244:GLU:CD	1:A:244:GLU:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ARG:HD3	1:B:484:ARG:OXT	2.13	0.48
1:F:172:SER:HB2	3:F:506:HOH:O	2.12	0.48
1:A:53:VAL:HG11	1:A:117:SER:N	2.29	0.48
1:A:210:VAL:HG23	1:A:211:ASP:N	2.28	0.48
1:D:134:LEU:HB3	1:D:138:MSE:HB3	1.94	0.48
1:F:190:THR:HG21	1:F:192:THR:HB	1.88	0.48
1:B:69:PRO:O	1:B:76:ARG:HD2	2.13	0.48
1:B:442:ASN:ND2	1:B:445:TYR:HB2	2.28	0.48
1:C:208:ARG:HD3	1:C:446:GLU:OE1	2.14	0.48
1:F:247:GLU:C	1:F:249:ALA:H	2.16	0.48
1:A:247:GLU:C	1:A:249:ALA:H	2.16	0.48
1:A:398:ARG:HD3	1:F:477:THR:HG22	1.95	0.48
1:C:53:VAL:HG12	1:C:54:TYR:O	2.13	0.48
1:D:369:ARG:HH11	1:D:369:ARG:HG2	1.78	0.48
1:E:16:LYS:HD3	1:E:114:VAL:HB	1.96	0.48
1:E:123:TYR:O	1:E:126:VAL:HG22	2.14	0.48
1:E:244:GLU:N	1:E:244:GLU:CD	2.67	0.48
1:E:453:LEU:O	1:E:457:ILE:HG13	2.14	0.48
1:F:321:ALA:HB3	1:F:422:THR:HB	1.95	0.48
1:A:8:LEU:HD11	1:A:12:GLN:CB	2.44	0.48
1:D:192:THR:CG2	1:D:193:PRO:N	2.77	0.48
1:E:210:VAL:HG23	1:E:211:ASP:N	2.29	0.48
1:E:430:PRO:HA	1:E:435:ILE:HG12	1.96	0.48
1:A:61:TRP:CE3	1:A:63:GLY:HA2	2.49	0.48
1:A:256:LYS:HE3	1:B:207:THR:OG1	2.14	0.48
1:A:356:LYS:HG3	1:A:366:VAL:HG11	1.96	0.48
1:B:56:SER:HB3	1:B:115:GLN:O	2.13	0.48
1:B:192:THR:HG23	1:B:193:PRO:HD2	1.94	0.48
1:D:346:GLU:CD	1:D:346:GLU:H	2.17	0.48
1:F:469:ARG:HG2	1:F:469:ARG:NH1	2.29	0.48
1:A:69:PRO:O	1:A:76:ARG:HD2	2.14	0.48
1:A:133:THR:HB	1:B:443:ARG:CD	2.44	0.48
1:B:53:VAL:HG13	1:B:117:SER:OG	2.14	0.48
1:C:346:GLU:CD	1:C:346:GLU:H	2.17	0.48
1:F:269:ASP:OD1	1:F:269:ASP:N	2.47	0.48
1:F:472:SER:OG	1:F:474:LYS:HG3	2.13	0.48
1:C:280:VAL:HA	1:C:405:GLU:OE2	2.14	0.48
1:D:361:ARG:HE	1:D:365:GLU:HG2	1.77	0.48
1:A:36:ILE:HG23	1:A:138:MSE:HE2	1.95	0.47
1:B:9:THR:HG23	1:B:12:GLN:HE21	1.78	0.47
1:B:27:ALA:HB1	1:B:51:LEU:HD21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ARG:HG3	1:C:187:ARG:NH1	2.28	0.47
1:D:46:ALA:O	1:D:51:LEU:HB2	2.14	0.47
1:D:428:ASP:HB3	1:D:436:LYS:HB2	1.95	0.47
1:B:210:VAL:HG23	1:B:211:ASP:N	2.29	0.47
1:B:321:ALA:HB3	1:B:422:THR:HB	1.96	0.47
1:D:356:LYS:HE2	1:D:363:GLY:O	2.14	0.47
1:A:16:LYS:HD3	1:A:114:VAL:HB	1.95	0.47
1:C:204:THR:HG22	1:C:303:ILE:O	2.15	0.47
1:C:441:ALA:HB3	1:D:131:GLU:HB2	1.96	0.47
1:D:381:ARG:HG3	1:D:381:ARG:O	2.14	0.47
1:E:51:LEU:HD22	1:E:52:PHE:CE2	2.50	0.47
1:A:210:VAL:CG2	1:A:211:ASP:N	2.76	0.47
1:B:56:SER:HB2	1:B:117:SER:HB3	1.96	0.47
1:B:326:ARG:HG2	1:B:326:ARG:NH1	2.28	0.47
1:C:210:VAL:HG23	1:C:211:ASP:N	2.28	0.47
1:D:134:LEU:HB3	1:D:138:MSE:HB2	1.96	0.47
1:F:151:LEU:HD22	1:F:151:LEU:N	2.29	0.47
1:F:360:GLY:O	1:F:361:ARG:C	2.52	0.47
1:A:28:LEU:HD13	1:A:126:VAL:HG21	1.96	0.47
1:C:173:HIS:CE1	1:C:480:GLU:OE2	2.68	0.47
1:E:361:ARG:HB2	1:E:361:ARG:CZ	2.42	0.47
1:A:427:SER:O	1:A:442:ASN:ND2	2.47	0.47
1:B:296:ARG:NH1	1:B:484:ARG:O	2.48	0.47
1:C:131:GLU:HG2	1:D:441:ALA:HB1	1.97	0.47
1:E:9:THR:HG23	1:E:12:GLN:HE21	1.80	0.47
1:F:313:GLN:HB2	1:F:429:LYS:NZ	2.29	0.47
1:C:8:LEU:HD12	1:C:9:THR:N	2.30	0.47
1:D:210:VAL:CG2	1:D:211:ASP:N	2.77	0.47
1:F:9:THR:CG2	1:F:12:GLN:HE21	2.28	0.47
1:F:309:LEU:N	1:F:313:GLN:HE22	2.12	0.47
1:F:326:ARG:NH2	1:F:335:LEU:O	2.48	0.47
1:B:210:VAL:CG2	1:B:211:ASP:N	2.78	0.47
1:D:451:GLU:O	1:D:455:ILE:HG13	2.15	0.47
1:B:189:TYR:HB3	1:B:260:MSE:HE3	1.97	0.47
1:C:244:GLU:CD	1:C:244:GLU:H	2.18	0.47
1:D:296:ARG:HD3	1:D:484:ARG:OXT	2.15	0.47
1:E:69:PRO:O	1:E:76:ARG:HD2	2.15	0.47
1:F:177:ARG:HG3	1:F:177:ARG:NH1	2.29	0.47
1:F:369:ARG:HG2	1:F:369:ARG:NH1	2.30	0.47
1:A:56:SER:HB3	1:A:115:GLN:O	2.15	0.47
1:B:54:TYR:CD2	1:B:176:ALA:HB1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:TYR:CG	1:D:124:PRO:HD3	2.49	0.47
1:F:190:THR:HG22	1:F:192:THR:N	2.30	0.47
1:B:244:GLU:CD	1:B:244:GLU:H	2.17	0.46
1:C:177:ARG:HG3	1:C:177:ARG:HH11	1.80	0.46
1:C:442:ASN:ND2	1:C:445:TYR:HB2	2.30	0.46
1:E:200:PHE:CD1	1:E:200:PHE:N	2.83	0.46
1:E:305:HIS:HB2	1:E:427:SER:HB3	1.97	0.46
1:F:29:ARG:HH21	1:F:128:ASP:HB2	1.79	0.46
1:B:150:GLU:C	1:B:151:LEU:HD22	2.35	0.46
1:C:129:GLY:O	1:C:130:SER:C	2.54	0.46
1:C:237:ASN:ND2	1:C:248:GLU:HB2	2.30	0.46
1:C:356:LYS:HE2	1:C:363:GLY:O	2.14	0.46
1:D:310:ARG:O	1:D:429:LYS:NZ	2.45	0.46
1:B:9:THR:HB	1:B:10:PRO:CD	2.44	0.46
1:C:244:GLU:HB2	1:C:245:ALA:H	1.54	0.46
1:C:359:SER:C	1:C:360:GLY:O	2.49	0.46
1:F:134:LEU:HB3	1:F:138:MSE:HB2	1.97	0.46
1:F:248:GLU:H	1:F:248:GLU:CD	2.18	0.46
1:B:346:GLU:CD	1:B:346:GLU:H	2.19	0.46
1:C:210:VAL:CG2	1:C:211:ASP:N	2.77	0.46
1:C:326:ARG:NH2	1:C:335:LEU:O	2.49	0.46
1:D:206:TYR:HB3	1:D:209:TYR:CD2	2.51	0.46
1:E:451:GLU:O	1:E:455:ILE:HG13	2.16	0.46
1:D:77:PHE:CE2	1:D:104:LEU:HD22	2.51	0.46
1:F:216:TRP:CZ3	1:F:265:LEU:HD12	2.50	0.46
1:D:61:TRP:CE3	1:D:63:GLY:HA2	2.50	0.46
1:F:310:ARG:O	1:F:429:LYS:NZ	2.43	0.46
1:B:190:THR:HG22	1:B:192:THR:N	2.30	0.46
1:C:9:THR:HB	1:C:10:PRO:CD	2.46	0.46
1:C:248:GLU:H	1:C:248:GLU:CD	2.18	0.46
1:D:434:GLU:HG2	3:D:517:HOH:O	2.15	0.46
1:E:63:GLY:CA	1:E:80:ALA:HB2	2.43	0.46
1:E:286:LYS:NZ	1:E:290:ASP:OD1	2.44	0.46
1:F:9:THR:HG23	1:F:12:GLN:HE21	1.79	0.46
1:A:266:ILE:HG22	1:A:267:THR:N	2.31	0.46
1:B:54:TYR:CE2	1:B:176:ALA:HB1	2.51	0.46
1:A:253:LEU:HD13	1:B:252:ASP:OD1	2.15	0.46
1:C:177:ARG:HG3	1:C:177:ARG:NH1	2.31	0.46
1:D:173:HIS:HE1	1:D:480:GLU:OE2	1.98	0.46
1:E:83:TYR:HA	1:E:169:SER:O	2.15	0.46
1:E:210:VAL:O	1:E:214:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:69:PRO:O	1:F:76:ARG:HD2	2.16	0.46
1:A:63:GLY:CA	1:A:80:ALA:HB2	2.45	0.46
1:C:8:LEU:HD11	1:C:12:GLN:HB3	1.98	0.46
1:D:72:ARG:HH12	1:D:103:LEU:HD22	1.75	0.46
1:E:53:VAL:HG11	1:E:117:SER:N	2.31	0.46
1:E:123:TYR:CG	1:E:124:PRO:HD3	2.51	0.46
1:F:9:THR:HB	1:F:10:PRO:CD	2.46	0.45
1:F:150:GLU:OE1	1:F:150:GLU:N	2.48	0.45
1:F:237:ASN:ND2	1:F:248:GLU:HB2	2.32	0.45
1:F:427:SER:O	1:F:428:ASP:HB3	2.16	0.45
1:C:46:ALA:O	1:C:51:LEU:HB2	2.17	0.45
1:C:298:ASP:OD1	1:C:471:HIS:HE1	1.99	0.45
1:C:335:LEU:HD21	1:C:341:ILE:HD11	1.98	0.45
1:A:212:GLU:HG2	1:A:450:SER:HA	1.98	0.45
1:F:56:SER:HB2	1:F:117:SER:HB3	1.97	0.45
1:F:192:THR:CG2	1:F:264:HIS:HE2	2.19	0.45
1:F:204:THR:HG22	1:F:303:ILE:O	2.16	0.45
1:F:253:LEU:HD21	1:F:257:LYS:HE3	1.99	0.45
1:F:361:ARG:N	1:F:362:PRO:HD3	2.31	0.45
1:A:133:THR:CB	1:B:443:ARG:HD3	2.46	0.45
1:B:173:HIS:HE1	1:B:480:GLU:OE2	1.99	0.45
1:B:463:LEU:O	1:B:466:GLU:HB2	2.17	0.45
1:C:443:ARG:HH11	1:C:443:ARG:CG	2.30	0.45
1:E:336:PRO:HA	1:E:337:PRO:HD3	1.90	0.45
1:F:53:VAL:HG11	1:F:117:SER:O	2.17	0.45
1:F:210:VAL:CG2	1:F:211:ASP:N	2.80	0.45
1:A:237:ASN:ND2	1:A:248:GLU:HB2	2.31	0.45
1:E:53:VAL:HG12	1:E:54:TYR:O	2.16	0.45
1:E:390:SER:HB3	1:E:394:PHE:CE1	2.52	0.45
1:A:54:TYR:CD2	1:A:176:ALA:HB1	2.52	0.45
1:B:248:GLU:H	1:B:248:GLU:CD	2.20	0.45
1:C:437:LEU:N	1:C:437:LEU:HD12	2.32	0.45
1:E:8:LEU:HD23	1:E:113:SER:HA	1.98	0.45
1:E:247:GLU:C	1:E:249:ALA:H	2.20	0.45
1:F:216:TRP:HZ3	1:F:265:LEU:HD12	1.82	0.45
1:C:253:LEU:HD11	1:C:257:LYS:HE3	1.97	0.45
1:E:448:ALA:O	1:E:449:ILE:C	2.55	0.45
1:F:326:ARG:HG2	1:F:326:ARG:NH1	2.31	0.45
1:B:123:TYR:O	1:B:126:VAL:HG22	2.17	0.45
1:E:192:THR:HG23	1:E:193:PRO:HD2	1.99	0.45
1:E:433:GLY:HA3	1:F:148:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:212:GLU:HG2	1:F:450:SER:HA	1.99	0.45
1:A:54:TYR:CE2	1:A:176:ALA:HB1	2.52	0.45
1:A:206:TYR:HB3	1:A:209:TYR:HD2	1.82	0.45
1:B:94:ARG:HD2	3:B:514:HOH:O	2.15	0.45
1:C:435:ILE:CG2	1:D:185:ARG:HH22	2.29	0.45
1:E:324:TYR:HE1	1:E:406:SER:HB3	1.81	0.45
1:B:9:THR:OG1	1:B:12:GLN:HG3	2.17	0.44
1:F:244:GLU:N	1:F:244:GLU:CD	2.70	0.44
1:B:68:PRO:HB2	1:B:70:LYS:HE3	1.99	0.44
1:C:8:LEU:HD11	1:C:12:GLN:CB	2.47	0.44
1:C:206:TYR:HB3	1:C:209:TYR:CD2	2.53	0.44
1:F:63:GLY:CA	1:F:80:ALA:HB2	2.47	0.44
1:F:437:LEU:HD12	1:F:437:LEU:N	2.32	0.44
1:B:192:THR:HG23	1:B:193:PRO:CD	2.48	0.44
1:C:8:LEU:CD1	1:C:12:GLN:HB2	2.48	0.44
1:C:16:LYS:HD3	1:C:114:VAL:HB	1.97	0.44
1:D:8:LEU:HD23	1:D:113:SER:HA	1.98	0.44
1:D:369:ARG:HG2	1:D:369:ARG:NH1	2.32	0.44
1:E:151:LEU:HD21	1:F:430:PRO:O	2.17	0.44
1:E:269:ASP:OD1	1:E:269:ASP:N	2.50	0.44
1:A:134:LEU:HB3	1:A:138:MSE:HB3	2.00	0.44
1:A:244:GLU:N	1:A:244:GLU:OE2	2.48	0.44
1:C:77:PHE:CE2	1:C:104:LEU:HD22	2.52	0.44
1:D:56:SER:HB3	1:D:115:GLN:O	2.17	0.44
1:E:427:SER:O	1:E:428:ASP:HB3	2.17	0.44
1:F:29:ARG:NH2	1:F:128:ASP:HB2	2.33	0.44
1:B:28:LEU:HD13	1:B:126:VAL:CG2	2.46	0.44
1:C:9:THR:OG1	1:C:12:GLN:HG3	2.18	0.44
1:D:359:SER:HA	1:D:451:GLU:OE1	2.18	0.44
1:E:51:LEU:HD22	1:E:52:PHE:CD2	2.53	0.44
1:A:89:ARG:HH11	1:A:89:ARG:HB3	1.81	0.44
1:A:192:THR:CG2	1:A:193:PRO:N	2.80	0.44
1:A:398:ARG:CD	1:F:477:THR:HG22	2.47	0.44
1:A:443:ARG:HD3	1:B:133:THR:HG23	1.99	0.44
1:D:206:TYR:CE2	1:D:449:ILE:HD11	2.53	0.44
1:E:210:VAL:CG2	1:E:211:ASP:N	2.81	0.44
1:C:243:THR:O	1:C:244:GLU:C	2.56	0.44
1:C:324:TYR:CE1	1:C:406:SER:HB3	2.53	0.44
1:C:433:GLY:HA3	1:D:148:THR:HB	2.00	0.44
1:D:244:GLU:N	1:D:244:GLU:CD	2.71	0.44
1:E:9:THR:CG2	1:E:12:GLN:HE21	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:PHE:CE2	1:E:104:LEU:HD22	2.53	0.44
1:D:100:GLN:HB3	1:D:483:PHE:CD1	2.53	0.44
1:D:245:ALA:HB1	1:D:247:GLU:OE1	2.17	0.44
1:F:344:ILE:HG22	1:F:346:GLU:OE1	2.18	0.44
1:A:437:LEU:H	1:A:437:LEU:CD1	2.26	0.44
1:C:28:LEU:HD13	1:C:126:VAL:HG21	1.99	0.44
1:D:261:PRO:HB2	1:D:263:TRP:CZ3	2.53	0.44
1:D:326:ARG:NH2	1:D:335:LEU:O	2.51	0.44
1:F:253:LEU:HD21	1:F:257:LYS:CE	2.48	0.44
1:A:9:THR:HG22	1:A:105:TYR:OH	2.18	0.43
1:A:53:VAL:HG11	1:A:117:SER:O	2.18	0.43
1:B:463:LEU:HD22	1:B:470:LEU:HD13	2.00	0.43
1:D:182:SER:HB3	1:D:291:HIS:HA	2.00	0.43
1:F:182:SER:HB3	1:F:291:HIS:HA	1.99	0.43
1:F:201:VAL:HB	1:F:300:TRP:HB3	2.00	0.43
1:A:248:GLU:H	1:A:248:GLU:CD	2.17	0.43
1:C:206:TYR:HB3	1:C:209:TYR:HD2	1.83	0.43
1:C:386:ARG:O	1:C:387:TYR:C	2.57	0.43
1:D:361:ARG:O	1:D:366:VAL:HG13	2.18	0.43
1:D:477:THR:HG22	1:E:398:ARG:HD3	2.00	0.43
1:F:192:THR:CG2	1:F:193:PRO:N	2.80	0.43
1:A:68:PRO:HB2	1:A:70:LYS:HE3	2.00	0.43
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.79	0.43
1:A:353:ASP:O	1:A:357:LEU:HG	2.18	0.43
1:B:112:ILE:HG22	1:B:113:SER:N	2.33	0.43
1:F:8:LEU:HD11	1:F:12:GLN:CB	2.48	0.43
1:F:14:LEU:HD11	1:F:98:ASN:HB2	1.99	0.43
1:A:201:VAL:HB	1:A:300:TRP:HB3	2.00	0.43
1:B:83:TYR:HA	1:B:169:SER:O	2.19	0.43
1:E:204:THR:HG22	1:E:303:ILE:O	2.18	0.43
1:B:32:ILE:O	1:B:36:ILE:HG13	2.18	0.43
1:C:324:TYR:HE1	1:C:406:SER:HB3	1.83	0.43
1:D:63:GLY:CA	1:D:80:ALA:HB2	2.46	0.43
1:D:436:LYS:HG3	1:D:442:ASN:HD22	1.79	0.43
1:E:220:GLN:NE2	1:E:226:SER:OG	2.51	0.43
1:E:296:ARG:N	1:E:297:PRO:HD3	2.34	0.43
1:E:308:GLY:CA	1:E:313:GLN:NE2	2.81	0.43
1:F:65:THR:HB	1:F:68:PRO:HG3	2.01	0.43
1:F:192:THR:HG23	1:F:193:PRO:CD	2.47	0.43
1:F:435:ILE:HG22	1:F:435:ILE:O	2.19	0.43
1:A:189:TYR:HB3	1:A:260:MSE:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:HIS:HB2	1:A:427:SER:HB3	2.01	0.43
1:A:326:ARG:NH2	1:A:335:LEU:O	2.51	0.43
1:B:9:THR:CG2	1:B:12:GLN:HE21	2.32	0.43
1:C:9:THR:HG23	1:C:12:GLN:NE2	2.33	0.43
1:C:192:THR:HG23	1:C:193:PRO:CD	2.49	0.43
1:D:477:THR:HB	1:E:395:ASN:HD21	1.84	0.43
1:F:61:TRP:CE2	1:F:108:TYR:HD2	2.37	0.43
1:F:210:VAL:HG21	1:F:255:TRP:CH2	2.54	0.43
1:B:89:ARG:N	1:B:90:PRO:HD3	2.34	0.43
1:B:356:LYS:HE2	1:B:363:GLY:H	1.83	0.43
1:D:266:ILE:HG22	1:D:267:THR:N	2.33	0.43
1:E:65:THR:HB	1:E:68:PRO:HG3	2.00	0.43
1:E:212:GLU:HG2	1:E:450:SER:HA	2.00	0.43
1:F:206:TYR:CE2	1:F:449:ILE:HD11	2.53	0.43
1:B:265:LEU:HD23	1:B:265:LEU:HA	1.80	0.43
1:C:131:GLU:OE2	1:C:131:GLU:HA	2.17	0.43
1:C:396:LEU:HD12	1:C:396:LEU:HA	1.91	0.43
1:D:237:ASN:ND2	1:D:248:GLU:HB2	2.34	0.43
1:D:440:GLN:HB3	1:D:441:ALA:H	1.65	0.43
1:F:61:TRP:CE3	1:F:63:GLY:HA2	2.54	0.43
1:B:123:TYR:CG	1:B:124:PRO:HD3	2.54	0.43
1:F:480:GLU:HA	1:F:481:PRO:HD3	1.92	0.43
1:A:9:THR:HB	1:A:10:PRO:CD	2.48	0.43
1:C:326:ARG:HG2	1:C:326:ARG:NH1	2.32	0.43
1:C:427:SER:O	1:C:428:ASP:HB3	2.19	0.43
1:E:248:GLU:H	1:E:248:GLU:CD	2.22	0.43
1:F:9:THR:OG1	1:F:12:GLN:HG3	2.19	0.43
1:B:29:ARG:HH21	1:B:128:ASP:HB2	1.84	0.42
1:B:53:VAL:HG11	1:B:117:SER:N	2.33	0.42
1:B:364:GLU:HB3	1:C:469:ARG:NH2	2.31	0.42
1:C:63:GLY:CA	1:C:80:ALA:HB2	2.47	0.42
1:D:69:PRO:O	1:D:76:ARG:HD2	2.19	0.42
1:F:132:LEU:HD23	1:F:132:LEU:HA	1.85	0.42
1:F:361:ARG:HB2	1:F:361:ARG:HH11	1.84	0.42
1:A:259:GLN:C	1:A:260:MSE:HG3	2.38	0.42
1:B:61:TRP:CE3	1:B:63:GLY:HA2	2.53	0.42
1:B:63:GLY:CA	1:B:80:ALA:HB2	2.49	0.42
1:B:206:TYR:CE2	1:B:449:ILE:HD11	2.54	0.42
1:B:363:GLY:C	1:B:365:GLU:H	2.22	0.42
1:B:395:ASN:ND2	1:C:478:PHE:HD1	2.14	0.42
1:C:347:VAL:HG12	1:C:351:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:TYR:OH	1:D:483:PHE:HB3	2.19	0.42
1:D:377:THR:HA	1:D:403:ASP:O	2.19	0.42
1:E:54:TYR:CE2	1:E:176:ALA:HB1	2.53	0.42
1:E:89:ARG:N	1:E:90:PRO:HD3	2.34	0.42
1:E:189:TYR:O	1:E:258:HIS:HB3	2.20	0.42
1:E:334:VAL:CG1	1:F:386:ARG:HD2	2.49	0.42
1:F:150:GLU:OE1	1:F:150:GLU:O	2.38	0.42
1:A:46:ALA:O	1:A:51:LEU:HB2	2.19	0.42
1:D:127:ILE:HD13	1:D:132:LEU:CG	2.47	0.42
1:D:330:VAL:HG22	1:D:330:VAL:O	2.20	0.42
1:F:336:PRO:HA	1:F:337:PRO:HD3	1.89	0.42
1:F:347:VAL:HG12	1:F:351:LEU:CD2	2.49	0.42
1:F:392:LEU:O	1:F:396:LEU:HB2	2.18	0.42
1:A:29:ARG:NH2	1:A:128:ASP:HB2	2.35	0.42
1:B:469:ARG:NH1	1:B:469:ARG:CG	2.81	0.42
1:B:477:THR:HB	1:C:395:ASN:HD21	1.83	0.42
1:E:54:TYR:CE1	1:E:121:ILE:HA	2.54	0.42
1:A:334:VAL:CG1	1:B:386:ARG:HD2	2.50	0.42
1:C:8:LEU:HD12	1:C:12:GLN:HB2	2.02	0.42
1:F:53:VAL:HG11	1:F:117:SER:N	2.35	0.42
1:D:190:THR:HG22	1:D:192:THR:CB	2.43	0.42
1:B:36:ILE:HA	1:B:138:MSE:CE	2.43	0.42
1:E:56:SER:HB2	1:E:117:SER:HB3	2.01	0.42
1:E:305:HIS:HB3	1:E:445:TYR:OH	2.20	0.42
1:F:296:ARG:N	1:F:297:PRO:HD3	2.35	0.42
1:A:83:TYR:HA	1:A:169:SER:O	2.20	0.42
1:A:228:TYR:CD1	1:A:265:LEU:HD13	2.55	0.42
1:B:243:THR:O	1:B:244:GLU:C	2.57	0.42
1:C:451:GLU:O	1:C:455:ILE:HG13	2.20	0.42
1:D:305:HIS:HB3	1:D:445:TYR:OH	2.20	0.42
1:E:280:VAL:HA	1:E:405:GLU:OE2	2.20	0.42
1:E:298:ASP:O	1:E:299:VAL:HB	2.20	0.42
1:E:353:ASP:O	1:E:357:LEU:HG	2.20	0.42
1:A:173:HIS:CD2	1:A:296:ARG:NH1	2.88	0.42
1:A:190:THR:HG22	1:A:192:THR:N	2.34	0.42
1:A:395:ASN:HD21	1:F:477:THR:HB	1.85	0.42
1:D:53:VAL:HG13	1:D:117:SER:OG	2.20	0.42
1:E:326:ARG:HG2	1:E:326:ARG:NH1	2.33	0.42
1:B:259:GLN:C	1:B:260:MSE:HG3	2.39	0.42
1:B:432:HIS:O	1:B:434:GLU:N	2.50	0.42
1:D:437:LEU:HD12	1:D:437:LEU:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:LEU:HA	1:D:466:GLU:HG3	2.02	0.42
1:F:14:LEU:HD13	1:F:94:ARG:HD3	2.02	0.42
1:B:264:HIS:CE1	1:B:274:THR:HG23	2.55	0.41
1:C:133:THR:HG22	1:D:443:ARG:HD2	2.02	0.41
1:C:247:GLU:C	1:C:249:ALA:N	2.74	0.41
1:D:242:GLU:O	1:D:242:GLU:HG2	2.20	0.41
1:D:264:HIS:CE1	1:D:274:THR:HG23	2.55	0.41
1:D:305:HIS:HB2	1:D:427:SER:HB3	2.02	0.41
1:E:296:ARG:NH1	1:E:484:ARG:O	2.53	0.41
1:E:346:GLU:CD	1:E:346:GLU:H	2.23	0.41
1:F:142:LEU:HD23	1:F:146:PHE:CD2	2.54	0.41
1:F:181:PHE:O	1:F:185:ARG:HD3	2.20	0.41
1:F:305:HIS:HB2	1:F:427:SER:HB3	2.02	0.41
1:F:466:GLU:O	1:F:469:ARG:HB2	2.20	0.41
1:A:243:THR:O	1:A:244:GLU:C	2.58	0.41
1:A:252:ASP:OD1	1:B:253:LEU:HD13	2.20	0.41
1:B:369:ARG:HG2	1:B:369:ARG:HH11	1.84	0.41
1:C:298:ASP:OD1	1:C:471:HIS:CE1	2.74	0.41
1:D:336:PRO:HA	1:D:337:PRO:HD3	1.94	0.41
1:D:347:VAL:HG12	1:D:351:LEU:HD22	2.01	0.41
1:F:440:GLN:CG	1:F:441:ALA:N	2.80	0.41
1:A:190:THR:HG23	1:A:262:ALA:CB	2.46	0.41
1:D:28:LEU:HD13	1:D:126:VAL:CG2	2.51	0.41
1:D:52:PHE:O	1:D:121:ILE:HG13	2.20	0.41
1:E:29:ARG:NH2	1:E:128:ASP:HB2	2.35	0.41
1:E:185:ARG:HG3	1:F:437:LEU:HD21	2.01	0.41
1:E:192:THR:HG23	1:E:193:PRO:CD	2.50	0.41
1:D:9:THR:HG23	1:D:12:GLN:HE21	1.84	0.41
1:F:8:LEU:HD12	1:F:12:GLN:HB2	2.02	0.41
1:A:187:ARG:HG3	1:A:187:ARG:NH1	2.32	0.41
1:A:288:ILE:HG23	1:A:289:CYS:N	2.36	0.41
1:B:192:THR:CG2	1:B:193:PRO:N	2.83	0.41
1:C:251:SER:HA	3:C:507:HOH:O	2.20	0.41
1:D:206:TYR:HB3	1:D:209:TYR:HD2	1.85	0.41
1:E:29:ARG:HH21	1:E:128:ASP:HB2	1.86	0.41
1:E:411:ALA:O	1:E:414:TYR:HB3	2.21	0.41
1:A:8:LEU:HD11	1:A:12:GLN:HB3	2.01	0.41
1:B:133:THR:HG22	1:B:133:THR:O	2.21	0.41
1:C:244:GLU:N	1:C:244:GLU:OE2	2.52	0.41
1:D:53:VAL:HG11	1:D:117:SER:O	2.20	0.41
1:D:298:ASP:OD1	1:D:471:HIS:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ARG:NH1	1:E:177:ARG:HG3	2.36	0.41
1:F:123:TYR:CG	1:F:124:PRO:HD3	2.56	0.41
1:F:189:TYR:HB3	1:F:260:MSE:HE3	2.02	0.41
1:F:259:GLN:C	1:F:260:MSE:HG3	2.41	0.41
1:F:265:LEU:HD23	1:F:265:LEU:HA	1.74	0.41
1:F:298:ASP:OD1	1:F:471:HIS:HE1	2.04	0.41
1:C:8:LEU:CD1	1:C:12:GLN:CB	2.99	0.41
1:C:79:HIS:CE1	1:C:83:TYR:OH	2.73	0.41
1:C:101:LEU:HD23	1:C:101:LEU:HA	1.93	0.41
1:E:377:THR:HB	1:E:407:ALA:HB3	2.03	0.41
1:C:181:PHE:O	1:C:185:ARG:HD3	2.21	0.41
1:E:89:ARG:HB3	1:E:89:ARG:HH11	1.85	0.41
1:F:206:TYR:OH	1:F:439:GLY:HA2	2.20	0.41
1:F:362:PRO:O	1:F:365:GLU:HB3	2.21	0.41
1:A:181:PHE:O	1:A:185:ARG:HD3	2.21	0.41
1:A:216:TRP:CZ3	1:A:265:LEU:HD12	2.56	0.41
1:C:436:LYS:C	1:C:437:LEU:HD12	2.40	0.41
1:D:206:TYR:HE2	1:D:449:ILE:HD11	1.86	0.41
1:D:216:TRP:CZ3	1:D:265:LEU:HD12	2.56	0.41
1:D:259:GLN:C	1:D:260:MSE:HG3	2.40	0.41
1:F:8:LEU:HD11	1:F:12:GLN:HB2	2.02	0.41
1:F:200:PHE:CD1	1:F:200:PHE:N	2.88	0.41
1:F:202:LEU:CD1	1:F:460:ILE:HD11	2.38	0.41
1:A:9:THR:HG23	1:A:12:GLN:HE21	1.86	0.41
1:A:377:THR:HA	1:A:403:ASP:O	2.21	0.41
1:D:54:TYR:CD2	1:D:176:ALA:HB1	2.56	0.41
1:D:65:THR:HB	1:D:68:PRO:HG3	2.01	0.41
1:A:8:LEU:HD11	1:A:12:GLN:HB2	2.04	0.40
1:C:192:THR:CG2	1:C:193:PRO:N	2.83	0.40
1:C:437:LEU:HA	1:C:438:PRO:HD3	1.91	0.40
1:D:132:LEU:HB3	1:D:134:LEU:CD1	2.51	0.40
1:E:309:LEU:H	1:E:313:GLN:HE22	1.69	0.40
1:B:216:TRP:CZ3	1:B:265:LEU:HD12	2.57	0.40
1:B:478:PHE:N	1:C:395:ASN:HD21	2.13	0.40
1:C:151:LEU:CD2	1:D:431:LEU:HA	2.51	0.40
1:C:248:GLU:HA	3:C:507:HOH:O	2.21	0.40
1:C:328:ASP:O	1:C:330:VAL:N	2.48	0.40
1:E:187:ARG:HG3	1:E:187:ARG:NH1	2.36	0.40
1:E:364:GLU:H	1:E:364:GLU:CD	2.24	0.40
1:F:266:ILE:HG22	1:F:267:THR:N	2.37	0.40
1:A:8:LEU:HD12	1:A:12:GLN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:LEU:CD1	1:A:12:GLN:CB	2.99	0.40
1:A:427:SER:O	1:A:428:ASP:HB3	2.21	0.40
1:B:378:THR:O	1:B:404:MSE:HG2	2.22	0.40
1:D:243:THR:O	1:D:244:GLU:C	2.59	0.40
1:E:177:ARG:HG3	1:E:177:ARG:HH11	1.86	0.40
1:A:151:LEU:N	1:A:151:LEU:HD22	2.36	0.40
1:A:305:HIS:CE1	1:A:438:PRO:HG2	2.57	0.40
1:C:14:LEU:HD13	1:C:94:ARG:HD3	2.04	0.40
1:D:216:TRP:HZ3	1:D:265:LEU:HD12	1.87	0.40
1:E:68:PRO:HB2	1:E:70:LYS:HE3	2.03	0.40
1:F:437:LEU:O	1:F:438:PRO:C	2.60	0.40
1:F:474:LYS:NZ	2:F:501:PO4:O1	2.53	0.40
1:B:53:VAL:HG12	1:B:54:TYR:O	2.22	0.40
1:C:68:PRO:HB2	1:C:70:LYS:HE3	2.03	0.40
1:C:136:ARG:CZ	1:D:444:PHE:CD2	3.05	0.40
1:C:443:ARG:HH11	1:C:443:ARG:HG3	1.85	0.40
1:D:8:LEU:HD12	1:D:12:GLN:HB2	2.04	0.40
1:D:8:LEU:CD1	1:D:12:GLN:HB2	2.51	0.40
1:D:32:ILE:O	1:D:36:ILE:HG13	2.21	0.40
1:D:53:VAL:HG11	1:D:117:SER:N	2.35	0.40
1:D:325:LEU:HD12	1:D:325:LEU:HA	1.92	0.40
1:E:28:LEU:O	1:E:32:ILE:HG13	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	457/484 (94%)	408 (89%)	39 (8%)	10 (2%)	6 31
1	B	457/484 (94%)	409 (90%)	38 (8%)	10 (2%)	6 31
1	C	457/484 (94%)	407 (89%)	41 (9%)	9 (2%)	7 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	457/484 (94%)	403 (88%)	42 (9%)	12 (3%)	5	27
1	E	457/484 (94%)	410 (90%)	37 (8%)	10 (2%)	6	31
1	F	457/484 (94%)	399 (87%)	50 (11%)	8 (2%)	8	37
All	All	2742/2904 (94%)	2436 (89%)	247 (9%)	59 (2%)	6	31

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	GLU
1	B	244	GLU
1	C	244	GLU
1	D	244	GLU
1	D	436	LYS
1	E	244	GLU
1	E	441	ALA
1	F	244	GLU
1	A	130	SER
1	A	406	SER
1	C	133	THR
1	C	406	SER
1	D	129	GLY
1	F	129	GLY
1	A	438	PRO
1	A	443	ARG
1	B	252	ASP
1	B	406	SER
1	E	299	VAL
1	E	433	GLY
1	A	433	GLY
1	B	10	PRO
1	B	129	GLY
1	B	251	SER
1	C	252	ASP
1	D	10	PRO
1	D	251	SER
1	D	252	ASP
1	D	329	HIS
1	D	406	SER
1	E	251	SER
1	E	252	ASP
1	E	443	ARG

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Mol	Chain	Res	Type
1	F	299	VAL
1	F	362	PRO
1	F	406	SER
1	A	10	PRO
1	A	251	SER
1	A	391	ALA
1	B	329	HIS
1	C	10	PRO
1	C	251	SER
1	D	391	ALA
1	D	435	ILE
1	E	10	PRO
1	E	406	SER
1	B	248	GLU
1	C	248	GLU
1	D	248	GLU
1	F	128	ASP
1	D	299	VAL
1	F	10	PRO
1	A	299	VAL
1	F	449	ILE
1	B	299	VAL
1	B	433	GLY
1	C	299	VAL
1	C	362	PRO
1	E	449	ILE

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	390/403 (97%)	369 (95%)	21 (5%)	22	57
1	B	390/403 (97%)	364 (93%)	26 (7%)	16	49
1	C	390/403 (97%)	368 (94%)	22 (6%)	21	56
1	D	390/403 (97%)	369 (95%)	21 (5%)	22	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	390/403 (97%)	367 (94%)	23 (6%)	19	54
1	F	390/403 (97%)	367 (94%)	23 (6%)	19	54
All	All	2340/2418 (97%)	2204 (94%)	136 (6%)	20	55

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	28	LEU
1	A	51	LEU
1	A	89	ARG
1	A	202	LEU
1	A	222	LEU
1	A	244	GLU
1	A	265	LEU
1	A	284	ASN
1	A	296	ARG
1	A	300	TRP
1	A	301	LEU
1	A	322	HIS
1	A	351	LEU
1	A	364	GLU
1	A	400	VAL
1	A	403	ASP
1	A	431	LEU
1	A	437	LEU
1	A	440	GLN
1	A	469	ARG
1	B	25	VAL
1	B	28	LEU
1	B	51	LEU
1	B	89	ARG
1	B	95	SER
1	B	148	THR
1	B	168	PHE
1	B	190	THR
1	B	202	LEU
1	B	207	THR
1	B	222	LEU
1	B	244	GLU
1	B	265	LEU

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Mol	Chain	Res	Type
1	B	284	ASN
1	B	300	TRP
1	B	301	LEU
1	B	322	HIS
1	B	351	LEU
1	B	361	ARG
1	B	364	GLU
1	B	400	VAL
1	B	431	LEU
1	B	437	LEU
1	B	438	PRO
1	B	443	ARG
1	B	469	ARG
1	C	25	VAL
1	C	28	LEU
1	C	51	LEU
1	C	89	ARG
1	C	131	GLU
1	C	132	LEU
1	C	151	LEU
1	C	202	LEU
1	C	207	THR
1	C	222	LEU
1	C	244	GLU
1	C	265	LEU
1	C	284	ASN
1	C	300	TRP
1	C	301	LEU
1	C	322	HIS
1	C	342	PRO
1	C	351	LEU
1	C	400	VAL
1	C	431	LEU
1	C	443	ARG
1	C	469	ARG
1	D	25	VAL
1	D	28	LEU
1	D	51	LEU
1	D	89	ARG
1	D	149	THR
1	D	168	PHE
1	D	190	THR

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Mol	Chain	Res	Type
1	D	202	LEU
1	D	222	LEU
1	D	244	GLU
1	D	265	LEU
1	D	284	ASN
1	D	296	ARG
1	D	300	TRP
1	D	301	LEU
1	D	322	HIS
1	D	351	LEU
1	D	364	GLU
1	D	400	VAL
1	D	437	LEU
1	D	469	ARG
1	E	25	VAL
1	E	28	LEU
1	E	51	LEU
1	E	89	ARG
1	E	95	SER
1	E	149	THR
1	E	168	PHE
1	E	190	THR
1	E	202	LEU
1	E	222	LEU
1	E	244	GLU
1	E	265	LEU
1	E	284	ASN
1	E	300	TRP
1	E	301	LEU
1	E	322	HIS
1	E	351	LEU
1	E	364	GLU
1	E	396	LEU
1	E	400	VAL
1	E	431	LEU
1	E	443	ARG
1	E	469	ARG
1	F	25	VAL
1	F	28	LEU
1	F	51	LEU
1	F	89	ARG
1	F	133	THR

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Mol	Chain	Res	Type
1	F	150	GLU
1	F	168	PHE
1	F	190	THR
1	F	202	LEU
1	F	207	THR
1	F	222	LEU
1	F	244	GLU
1	F	265	LEU
1	F	284	ASN
1	F	300	TRP
1	F	301	LEU
1	F	322	HIS
1	F	351	LEU
1	F	364	GLU
1	F	366	VAL
1	F	400	VAL
1	F	431	LEU
1	F	469	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	173	HIS
1	A	220	GLN
1	A	237	ASN
1	A	284	ASN
1	A	313	GLN
1	A	329	HIS
1	A	395	ASN
1	A	471	HIS
1	B	12	GLN
1	B	173	HIS
1	B	188	HIS
1	B	220	GLN
1	B	237	ASN
1	B	284	ASN
1	B	313	GLN
1	B	329	HIS
1	B	395	ASN
1	B	442	ASN
1	B	471	HIS

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Mol	Chain	Res	Type
1	C	12	GLN
1	C	173	HIS
1	C	188	HIS
1	C	220	GLN
1	C	237	ASN
1	C	284	ASN
1	C	313	GLN
1	C	329	HIS
1	C	395	ASN
1	C	440	GLN
1	C	442	ASN
1	C	471	HIS
1	D	12	GLN
1	D	173	HIS
1	D	188	HIS
1	D	220	GLN
1	D	237	ASN
1	D	284	ASN
1	D	313	GLN
1	D	329	HIS
1	D	395	ASN
1	D	442	ASN
1	D	471	HIS
1	E	12	GLN
1	E	173	HIS
1	E	188	HIS
1	E	220	GLN
1	E	237	ASN
1	E	284	ASN
1	E	313	GLN
1	E	329	HIS
1	E	395	ASN
1	E	440	GLN
1	E	471	HIS
1	F	12	GLN
1	F	173	HIS
1	F	188	HIS
1	F	220	GLN
1	F	237	ASN
1	F	284	ASN
1	F	313	GLN
1	F	329	HIS

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Mol	Chain	Res	Type
1	F	395	ASN
1	F	442	ASN
1	F	471	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	PO4	F	501	-	4,4,4	1.70	1 (25%)	6,6,6	0.47	0
2	PO4	B	503	-	4,4,4	1.77	2 (50%)	6,6,6	0.50	0
2	PO4	E	504	-	4,4,4	1.64	1 (25%)	6,6,6	0.51	0
2	PO4	D	505	-	4,4,4	1.85	2 (50%)	6,6,6	0.47	0
2	PO4	C	502	-	4,4,4	1.66	1 (25%)	6,6,6	0.50	0
2	PO4	A	506	-	4,4,4	1.62	0	6,6,6	0.47	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	505	PO4	P-O4	-2.42	1.47	1.54
2	F	501	PO4	P-O4	-2.27	1.48	1.54
2	C	502	PO4	P-O4	-2.24	1.48	1.54
2	B	503	PO4	P-O4	-2.15	1.48	1.54
2	E	504	PO4	P-O4	-2.15	1.48	1.54
2	D	505	PO4	P-O2	-2.13	1.48	1.54
2	B	503	PO4	P-O2	-2.07	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	PO4	1	0
2	E	504	PO4	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.