Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2016 – 06:51 PM EDT

PDB ID	:	5IZK
Title	:	The crystal structure of human eEFSec in complex with GDP
Authors	:	Dobosz-Bartoszek, M.; Simonovic, M.
Deposited on	:	2016-03-25
Resolution	:	3.25 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 ⓘ symbol.

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

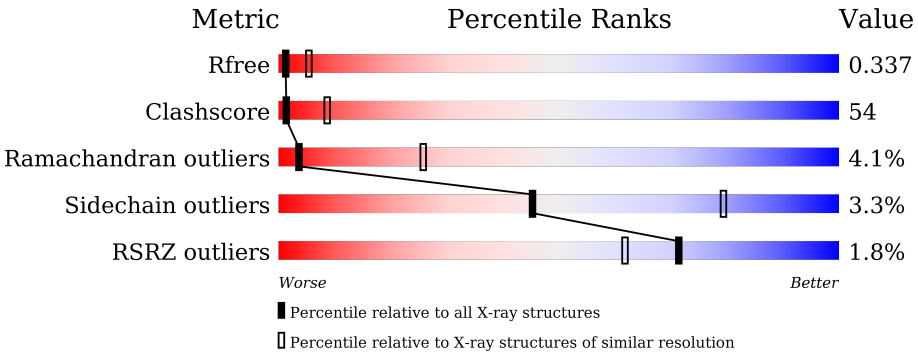
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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.

Mol	Chain	Length	Quality of chain
1	A	616	33% 41% · 22%
1	B	616	3% 41% 30% · 27%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6060 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 Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3216	2046	566	585	19			
1	B	451	Total	C	N	O	S	0	1	0
			2767	1746	499	514	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P57772
A	-18	GLY	-	expression tag	UNP P57772
A	-17	SER	-	expression tag	UNP P57772
A	-16	SER	-	expression tag	UNP P57772
A	-15	HIS	-	expression tag	UNP P57772
A	-14	HIS	-	expression tag	UNP P57772
A	-13	HIS	-	expression tag	UNP P57772
A	-12	HIS	-	expression tag	UNP P57772
A	-11	HIS	-	expression tag	UNP P57772
A	-10	HIS	-	expression tag	UNP P57772
A	-9	SER	-	expression tag	UNP P57772
A	-8	SER	-	expression tag	UNP P57772
A	-7	GLY	-	expression tag	UNP P57772
A	-6	LEU	-	expression tag	UNP P57772
A	-5	VAL	-	expression tag	UNP P57772
A	-4	PRO	-	expression tag	UNP P57772
A	-3	ARG	-	expression tag	UNP P57772
A	-2	GLY	-	expression tag	UNP P57772
A	-1	SER	-	expression tag	UNP P57772
A	0	HIS	-	expression tag	UNP P57772
B	-19	MET	-	initiating methionine	UNP P57772
B	-18	GLY	-	expression tag	UNP P57772
B	-17	SER	-	expression tag	UNP P57772
B	-16	SER	-	expression tag	UNP P57772
B	-15	HIS	-	expression tag	UNP P57772

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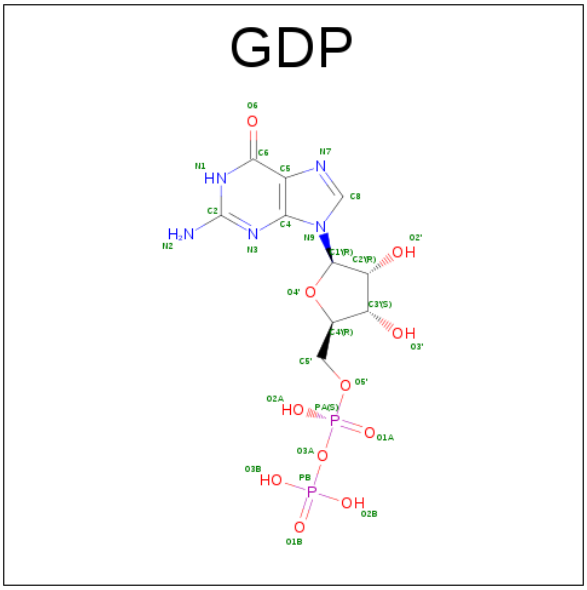
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P57772
B	-13	HIS	-	expression tag	UNP P57772
B	-12	HIS	-	expression tag	UNP P57772
B	-11	HIS	-	expression tag	UNP P57772
B	-10	HIS	-	expression tag	UNP P57772
B	-9	SER	-	expression tag	UNP P57772
B	-8	SER	-	expression tag	UNP P57772
B	-7	GLY	-	expression tag	UNP P57772
B	-6	LEU	-	expression tag	UNP P57772
B	-5	VAL	-	expression tag	UNP P57772
B	-4	PRO	-	expression tag	UNP P57772
B	-3	ARG	-	expression tag	UNP P57772
B	-2	GLY	-	expression tag	UNP P57772
B	-1	SER	-	expression tag	UNP P57772
B	0	HIS	-	expression tag	UNP P57772

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
2	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 3 is water.

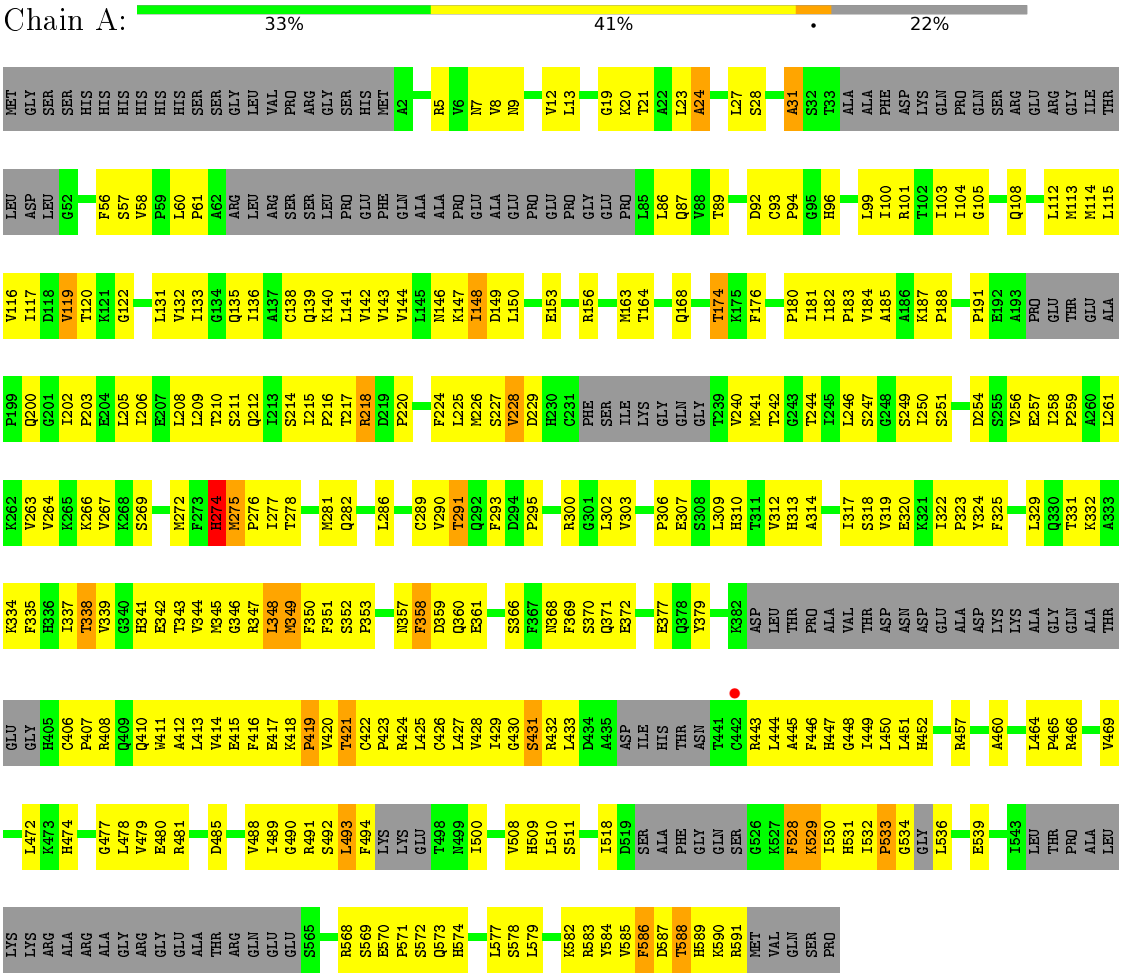
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total O 15 15	0	0
3	B	6	Total O 6 6	0	0

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.

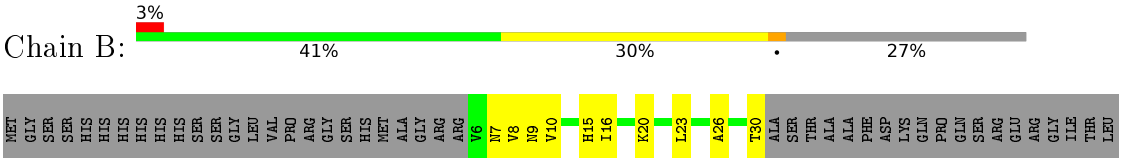
- Molecule 1: Selenocysteine-specific elongation factor

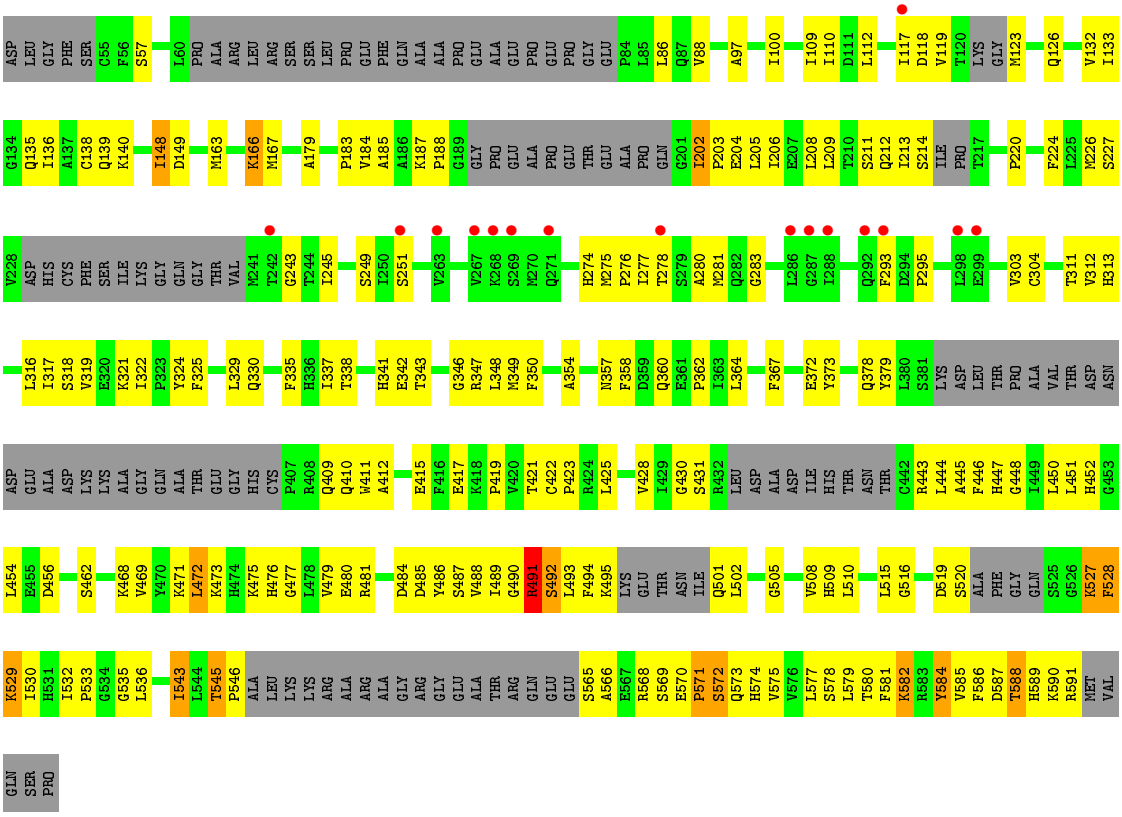
Chain A:



- Molecule 1: Selenocysteine-specific elongation factor

Chain B:




ASP LEU GLY PHE SER C55 F56 S57 L60 PRO ALA ARG LEU ARG SER SER LEU PRO GLU PHE GLN ALA ALA PRO GLU ALA GLU PRO GLU PRO GLY GLU P84 L85 L86 Q87 V88 A97 I100 I109 I110 D111 L112 I117 D118 V119 T120 LYS GLY M123 Q126 V132 I133
G134 Q135 I136 A137 C138 Q139 K140 I148 D149 M163 K166 M167 A179 P183 V184 A185 A186 K187 P188 G189 GLY PRO GLU ALA PRO GLU THR GLU ALA PRO GLN G201 I202 P203 E204 L205 I206 E207 L208 L209 T210 S211 Q212 I213 S214 ILE PRO T217 P220 F224 L225 M226 S227
V228 ASP HIS CYS PHE SER ILE LYS GLY GLN GLY THR VAL M241 T242 G243 T244 I245 S249 I250 S251 V263 V267 K268 S269 M270 Q271 H274 M275 P276 I277 T278 S279 A280 M281 Q282 G283 L286 G287 I288 Q292 F293 D294 P295 L298 E299 V303 C304 T311 V312 H313
L316 I317 S318 V319 E320 K321 I322 P323 Y324 F325 L329 Q330 F335 H336 I337 T338 H341 E342 T343 G346 R347 L348 M349 F350 A354 N357 F358 D359 Q360 E361 P362 I363 L364 F367 E372 Y373 Q378 Y379 L380 S381 LYS ASP LEU THR PRO ALA VAL THR ASP ASN
ASP GLU ALA ASP LYS LYS ALA GLY GLN ALA THR GLU GLY HIS CYS P407 R408 Q409 Q410 W411 A412 E415 F416 E417 K418 P419 V420 T421 C422 P423 R424 L425 V428 I429 G430 S431 R432 LEU ASP ALA ASP ILE HIS THR ASN THR C442 R443 L444 A445 F446 H447 G448 I449 L450 L451 H452 G453
L454 E455 D456 S462 K468 V469 Y470 K471 L472 K473 H474 K475 H476 G477 L478 V479 E480 R481 D484 D485 Y486 S487 V488 I489 G490 R491 S492 L493 F494 K495 LYS GLU THR ASN ILE Q501 L502 G505 V508 H509 L510 L515 G516 D519 S520 ALA PHE GLY GLN S525 G526 K527 F528
K529 I530 H531 I532 P533 G534 G535 L536 I543 L544 T545 P546 ALA LEU LYS LYS ARG ALA ARG ALA GLY ARG GLY GLU ALA THR ARG GLN GLU GLU S565 A566 E567 R568 S569 E570 P571 S572 Q573 H574 V575 V576 L577 S578 L579 T580 F581 K582 R583 Y584 V585 F586 D587 T588 H589 K590 R591 MET VAL
GLN SER PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.69Å 96.86Å 125.41Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	42.94 – 3.25 42.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.94-3.25) 91.2 (42.94-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.296 , 0.338 0.292 , 0.337	Depositor DCC
R_{free} test set	1097 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	89.2	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 71.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

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	0.36	0/3276	0.68	12/4477 (0.3%)
1	B	0.32	0/2816	0.66	8/3868 (0.2%)
All	All	0.34	0/6092	0.67	20/8345 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	464	LEU	N-CA-C	8.09	132.84	111.00
1	A	274	HIS	CB-CA-C	-7.73	94.93	110.40
1	B	565	SER	CB-CA-C	-7.32	96.19	110.10
1	B	341	HIS	N-CA-C	7.23	130.53	111.00
1	A	588	THR	N-CA-C	6.56	128.71	111.00
1	B	588	THR	N-CA-C	6.56	128.71	111.00
1	A	275	MET	N-CA-C	6.44	128.38	111.00
1	B	566	ALA	N-CA-CB	-6.25	101.34	110.10
1	B	582	LYS	N-CA-C	-6.15	94.40	111.00
1	A	214	SER	CB-CA-C	6.04	121.57	110.10
1	B	491	ARG	CB-CA-C	6.03	122.46	110.40
1	B	492	SER	N-CA-CB	5.88	119.33	110.50
1	A	338	THR	N-CA-C	-5.66	95.71	111.00
1	A	215	ILE	N-CA-C	5.49	125.83	111.00
1	B	529	LYS	CB-CA-C	5.42	121.23	110.40
1	A	349	MET	N-CA-C	-5.41	96.40	111.00
1	A	431	SER	N-CA-CB	-5.36	102.46	110.50
1	A	349	MET	CB-CA-C	5.20	120.80	110.40
1	A	215	ILE	C-N-CD	5.14	139.19	128.40
1	A	60	LEU	C-N-CD	5.04	138.99	128.40

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	3216	0	2771	331	0
1	B	2767	0	2027	258	0
2	A	28	0	12	4	0
2	B	28	0	12	7	0
3	A	15	0	0	19	0
3	B	6	0	0	10	0
All	All	6060	0	4822	583	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 54.

All (583) 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:477:GLY:HA2	1:B:492:SER:CB	1.25	1.59
1:B:477:GLY:CA	1:B:492:SER:CB	2.02	1.36
1:B:476:HIS:O	1:B:492:SER:CB	1.79	1.31
1:B:490:GLY:O	1:B:528:PHE:CD2	1.84	1.30
1:B:311:THR:CA	1:B:421:THR:HG22	1.65	1.24
1:A:588:THR:CG2	1:A:589:HIS:H	1.39	1.24
1:B:473:LYS:CD	1:B:579:LEU:HD21	1.71	1.20
1:B:473:LYS:HG2	1:B:579:LEU:CD1	1.72	1.19
1:B:473:LYS:CG	1:B:579:LEU:HD21	1.71	1.19
1:B:473:LYS:HG2	1:B:579:LEU:HD11	1.17	1.16
1:B:580:THR:HG23	1:B:590:LYS:HD3	1.18	1.16
1:B:205:LEU:O	1:B:209:LEU:HB2	1.48	1.14
1:B:20:LYS:N	2:B:1001:GDP:O1A	1.81	1.13
1:B:490:GLY:O	1:B:528:PHE:HD2	1.20	1.12
1:B:311:THR:CB	1:B:421:THR:HG22	1.79	1.12
1:B:372:GLU:CD	1:B:582:LYS:NZ	2.04	1.11
1:A:432:ARG:CB	1:A:443:ARG:O	1.99	1.11
1:B:311:THR:HA	1:B:421:THR:HG22	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLY:O	1:A:528:PHE:HB2	1.53	1.08
1:B:473:LYS:HG2	1:B:579:LEU:CG	1.83	1.07
1:A:588:THR:HG22	1:A:589:HIS:N	1.64	1.05
1:A:588:THR:HG22	1:A:589:HIS:H	0.95	1.05
1:B:580:THR:HG23	1:B:590:LYS:CD	1.87	1.03
1:A:433:LEU:HD12	1:A:433:LEU:O	1.59	1.01
1:B:347:ARG:HB2	1:B:415:GLU:HB2	1.43	1.00
1:A:583:ARG:N	3:A:1101:HOH:O	1.82	0.99
1:B:473:LYS:CG	1:B:579:LEU:CD2	2.40	0.99
1:A:469:VAL:O	3:A:1101:HOH:O	1.81	0.97
1:B:311:THR:HA	1:B:421:THR:CG2	1.95	0.96
1:B:187:LYS:O	2:B:1001:GDP:C6	2.17	0.96
1:B:543:ILE:HD13	1:B:571:PRO:HD2	1.48	0.96
1:A:113:MET:O	1:A:141:LEU:HG	1.66	0.95
1:B:322:ILE:HD13	1:B:444:LEU:HB3	1.47	0.95
1:A:226:MET:O	3:A:1102:HOH:O	1.85	0.93
1:B:311:THR:CB	1:B:421:THR:CG2	2.46	0.92
1:A:372:GLU:OE2	1:A:582:LYS:NZ	2.02	0.92
1:B:491:ARG:HA	1:B:528:PHE:CE2	2.05	0.91
1:A:302:LEU:HA	3:A:1102:HOH:O	1.70	0.91
1:B:473:LYS:CG	1:B:579:LEU:CG	2.49	0.91
1:A:153[B]:GLU:OE2	3:A:1103:HOH:O	1.88	0.90
1:A:478:LEU:O	3:A:1104:HOH:O	1.89	0.90
1:A:224:PHE:CD1	1:A:250:ILE:HD11	2.05	0.90
1:B:476:HIS:C	1:B:492:SER:CB	2.39	0.90
1:B:475:LYS:HD3	1:B:493:LEU:CB	2.02	0.90
1:B:471:LYS:N	1:B:581:PHE:O	2.05	0.90
1:B:428:VAL:N	1:B:448:GLY:O	2.05	0.89
1:B:491:ARG:HA	1:B:528:PHE:HE2	1.34	0.89
1:A:422:CYS:SG	3:A:1114:HOH:O	2.32	0.88
1:B:110:ILE:O	3:B:1101:HOH:O	1.92	0.88
1:B:431:SER:OG	1:B:445:ALA:N	2.07	0.88
1:A:250:ILE:HG22	1:A:251:SER:H	1.36	0.87
1:B:473:LYS:HG2	1:B:579:LEU:CD2	2.02	0.87
1:A:148:ILE:HG22	1:A:185:ALA:HB2	1.56	0.87
1:B:362:PRO:HA	1:B:409:GLN:NE2	1.90	0.86
1:A:144:VAL:HG12	1:A:182:ILE:HB	1.57	0.86
1:A:229:ASP:OD1	1:A:242:THR:O	1.95	0.85
1:A:224:PHE:CE1	1:A:250:ILE:HD11	2.12	0.84
1:B:473:LYS:HG2	1:B:579:LEU:HD21	1.58	0.84
1:A:359:ASP:HA	1:A:408:ARG:HG3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:HG23	1:A:589:HIS:H	1.40	0.84
1:A:588:THR:CG2	1:A:589:HIS:N	2.17	0.84
1:B:322:ILE:CD1	1:B:444:LEU:HB3	2.07	0.84
1:B:148:ILE:HD11	1:B:183:PRO:HB2	1.59	0.84
1:A:149:ASP:OD2	1:A:188:PRO:HA	1.79	0.83
1:B:480:GLU:HG2	1:B:481:ARG:HG2	1.58	0.83
1:B:57:SER:HA	1:B:86:LEU:O	1.78	0.83
1:B:473:LYS:CG	1:B:579:LEU:HD11	2.06	0.83
1:A:579:LEU:HA	1:A:590:LYS:HB2	1.60	0.82
1:B:16:ILE:O	3:B:1102:HOH:O	1.98	0.81
1:A:148:ILE:HG22	1:A:185:ALA:CB	2.11	0.81
1:A:488:VAL:HG12	1:A:489:ILE:H	1.45	0.81
1:A:335:PHE:HD1	1:A:431:SER:HA	1.46	0.81
1:A:205:LEU:O	1:A:209:LEU:HG	1.80	0.80
1:B:148:ILE:CD1	1:B:183:PRO:HB2	2.10	0.80
1:A:337:ILE:HA	1:A:430:GLY:HA3	1.62	0.80
1:A:570:GLU:OE1	3:A:1105:HOH:O	2.00	0.80
1:A:511:SER:N	1:A:574:HIS:O	2.16	0.79
1:A:258:ILE:HD12	1:A:261:LEU:HD21	1.64	0.79
1:A:13:LEU:HD21	1:A:113:MET:HE3	1.64	0.79
1:B:224:PHE:CD2	1:B:304:CYS:HA	2.18	0.79
1:A:490:GLY:O	1:A:528:PHE:CB	2.31	0.78
1:B:479:VAL:HB	1:B:573:GLN:CB	2.12	0.78
1:A:331:THR:HG23	1:A:349:MET:HA	1.66	0.78
1:A:510:LEU:O	3:A:1106:HOH:O	2.01	0.78
1:A:465:PRO:HA	1:A:584:TYR:HB2	1.65	0.78
1:A:220:PRO:HG3	1:A:281:MET:HE2	1.66	0.77
1:B:329:LEU:HD12	1:B:379:TYR:HD2	1.50	0.77
1:A:212:GLN:OE1	1:A:212:GLN:N	2.18	0.77
1:A:138:CYS:SG	1:A:139:GLN:N	2.58	0.76
1:A:587:ASP:O	1:A:588:THR:OG1	2.02	0.76
1:A:119:VAL:HG23	1:A:146:ASN:O	1.85	0.76
1:A:338:THR:O	1:A:429:ILE:O	2.02	0.76
1:A:342:GLU:OE1	1:A:418:LYS:NZ	2.15	0.76
1:B:485:ASP:OD1	1:B:536:LEU:HB2	1.86	0.75
1:A:153[A]:GLU:OE1	1:A:156:ARG:NH2	2.18	0.75
1:B:136:ILE:HD13	1:B:447:HIS:HB3	1.68	0.75
1:B:319:VAL:HG22	1:B:410:GLN:O	1.86	0.74
1:A:112:LEU:HD11	1:A:212:GLN:HB3	1.68	0.74
1:A:148:ILE:HG22	1:A:185:ALA:N	2.03	0.74
1:B:372:GLU:CD	1:B:582:LYS:HZ2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD11	1:A:302:LEU:HD22	1.69	0.73
1:A:351:PHE:CE1	1:A:411:TRP:HB2	2.22	0.73
1:B:317:ILE:HG22	1:B:450:LEU:HA	1.71	0.73
1:B:187:LYS:O	2:B:1001:GDP:N1	2.21	0.73
1:B:148:ILE:HG13	1:B:184:VAL:O	1.89	0.73
1:B:570:GLU:O	1:B:572:SER:N	2.21	0.73
1:A:266:LYS:O	1:A:290:VAL:HG13	1.88	0.72
1:A:112:LEU:HA	1:A:138:CYS:SG	2.30	0.72
1:A:413:LEU:HD23	1:A:413:LEU:O	1.90	0.72
1:A:310:HIS:CD2	1:A:312:VAL:CG2	2.72	0.72
1:A:13:LEU:HD21	1:A:113:MET:CE	2.20	0.72
1:B:431:SER:HB3	1:B:443:ARG:O	1.89	0.72
1:B:580:THR:CG2	1:B:590:LYS:HD3	2.10	0.72
1:A:113:MET:HB2	1:A:141:LEU:HD12	1.72	0.71
1:A:302:LEU:HD23	3:A:1102:HOH:O	1.90	0.71
1:B:477:GLY:N	1:B:492:SER:CB	2.52	0.71
1:B:588:THR:OG1	1:B:589:HIS:N	2.23	0.71
1:A:349:MET:O	1:A:412:ALA:HB1	1.90	0.71
1:B:10:VAL:HG13	1:B:112:LEU:O	1.91	0.71
1:A:105:GLY:HA3	1:A:341:HIS:CE1	2.26	0.70
1:A:246:LEU:O	1:A:282:GLN:NE2	2.19	0.70
1:A:101:ARG:HD2	1:A:341:HIS:O	1.90	0.70
1:B:473:LYS:CG	1:B:579:LEU:HG	2.22	0.70
1:B:570:GLU:OE2	3:B:1103:HOH:O	2.10	0.70
1:A:322:ILE:N	1:A:445:ALA:O	2.20	0.70
1:A:313:HIS:CD2	1:A:419:PRO:HB3	2.27	0.69
1:A:148:ILE:CG2	1:A:185:ALA:HB2	2.21	0.69
1:A:366:SER:O	1:A:451:LEU:HD13	1.92	0.69
1:B:490:GLY:C	1:B:528:PHE:CD2	2.66	0.69
1:A:249:SER:O	1:A:250:ILE:HD13	1.92	0.69
1:B:293:PHE:O	1:B:295:PRO:HD3	1.93	0.69
1:B:275:MET:N	1:B:276:PRO:HD2	2.08	0.68
1:A:220:PRO:HD3	1:A:281:MET:HE1	1.74	0.68
1:A:5:ARG:HH12	1:A:272:MET:C	1.96	0.68
1:A:528:PHE:C	1:A:529:LYS:HG3	2.14	0.68
1:B:274:HIS:C	1:B:276:PRO:HD2	2.14	0.68
1:A:310:HIS:CD2	1:A:312:VAL:HG23	2.27	0.68
1:A:117:ILE:O	1:A:146:ASN:N	2.26	0.68
1:A:228:VAL:HG12	1:A:300:ARG:HA	1.73	0.67
1:A:23:LEU:HD23	1:A:23:LEU:O	1.95	0.67
1:A:348:LEU:HD23	1:A:350:PHE:CZ	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ILE:HD11	1:A:319:VAL:HG22	1.76	0.67
1:B:148:ILE:H	1:B:185:ALA:HB2	1.60	0.67
1:A:293:PHE:O	1:A:295:PRO:HD3	1.95	0.67
1:B:187:LYS:N	2:B:1001:GDP:O6	2.27	0.67
1:A:274:HIS:C	1:A:276:PRO:HD2	2.15	0.67
1:B:149:ASP:OD2	1:B:188:PRO:HA	1.95	0.67
1:B:580:THR:O	1:B:588:THR:HG23	1.95	0.67
1:B:338:THR:HA	1:B:342:GLU:O	1.94	0.67
1:B:354:ALA:O	1:B:358:PHE:N	2.28	0.67
1:A:250:ILE:HG22	1:A:251:SER:N	2.09	0.66
1:A:103:ILE:CD1	1:A:113:MET:HE1	2.25	0.66
1:A:224:PHE:HA	1:A:247:SER:O	1.95	0.66
1:A:480:GLU:HG3	1:A:481:ARG:H	1.61	0.66
1:A:570:GLU:HG3	1:A:570:GLU:O	1.96	0.65
1:B:373:TYR:O	1:B:469:VAL:HA	1.96	0.65
1:B:486:TYR:HD1	1:B:535:GLY:HA2	1.61	0.65
1:A:310:HIS:CE1	1:A:424:ARG:HG2	2.32	0.65
1:B:322:ILE:HG13	1:B:446:PHE:HA	1.79	0.65
1:B:224:PHE:O	1:B:304:CYS:HB2	1.97	0.65
1:B:473:LYS:HG3	1:B:579:LEU:HG	1.78	0.64
1:A:335:PHE:CD1	1:A:431:SER:HA	2.31	0.64
1:A:122:GLY:HA2	1:A:163:MET:CE	2.28	0.64
1:A:417:GLU:HG3	1:A:418:LYS:N	2.11	0.64
1:A:13:LEU:HD11	1:A:113:MET:CE	2.27	0.64
1:A:431:SER:HB2	1:A:445:ALA:CB	2.28	0.64
1:A:491:ARG:N	3:A:1104:HOH:O	2.06	0.64
1:B:245:ILE:O	1:B:283:GLY:N	2.26	0.64
1:B:312:VAL:HG13	1:B:454:LEU:O	1.98	0.64
1:B:133:ILE:HG13	1:B:444:LEU:HD11	1.80	0.64
1:A:585:VAL:HG22	1:A:586:PHE:N	2.11	0.63
1:B:372:GLU:HA	1:B:468:LYS:O	1.98	0.63
1:B:580:THR:CG2	1:B:590:LYS:CD	2.69	0.63
1:A:578:SER:O	1:A:590:LYS:HG2	1.97	0.63
1:B:148:ILE:O	1:B:148:ILE:HG22	1.98	0.63
1:A:335:PHE:O	1:A:345:MET:HG3	1.99	0.63
1:A:570:GLU:O	1:A:572:SER:N	2.31	0.63
1:B:321:LYS:H	1:B:379:TYR:HE2	1.46	0.63
1:B:585:VAL:HG22	1:B:586:PHE:N	2.11	0.63
1:A:428:VAL:O	1:A:429:ILE:HG13	1.99	0.62
1:A:112:LEU:CD1	1:A:212:GLN:HB3	2.27	0.62
1:B:501:GLN:C	1:B:502:LEU:HD12	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:N	2:A:1001:GDP:O2A	2.32	0.62
1:A:92:ASP:OD1	1:A:93:CYS:N	2.24	0.62
1:A:274:HIS:HB3	1:A:276:PRO:HD2	1.81	0.62
1:A:372:GLU:CD	1:A:582:LYS:NZ	2.53	0.62
1:B:220:PRO:HB2	1:B:249:SER:HB2	1.82	0.62
1:A:359:ASP:HA	1:A:408:ARG:CG	2.27	0.62
1:B:224:PHE:HD2	1:B:304:CYS:HA	1.62	0.62
1:B:372:GLU:OE1	1:B:582:LYS:NZ	2.32	0.62
1:B:372:GLU:CD	1:B:582:LYS:HZ1	1.80	0.62
1:A:431:SER:OG	1:A:444:LEU:HA	1.98	0.62
1:A:57:SER:HA	1:A:86:LEU:O	1.99	0.62
1:A:257:GLU:OE2	1:A:306:PRO:HA	2.00	0.61
1:B:372:GLU:OE2	1:B:582:LYS:NZ	2.15	0.61
1:A:450:LEU:HD23	1:A:452:HIS:H	1.64	0.61
1:A:539:GLU:OE1	1:A:539:GLU:N	2.32	0.61
1:B:338:THR:CB	1:B:343:THR:HG22	2.30	0.61
1:A:21:THR:HB	2:A:1001:GDP:O1A	2.01	0.61
1:B:203:PRO:O	1:B:206:ILE:N	2.34	0.61
1:A:488:VAL:HG12	1:A:489:ILE:N	2.16	0.61
1:B:472:LEU:O	1:B:472:LEU:HD23	2.01	0.61
1:B:456:ASP:OD2	1:B:462:SER:CB	2.48	0.60
1:A:251:SER:HA	1:A:278:THR:O	2.00	0.60
1:B:491:ARG:CA	1:B:528:PHE:CE2	2.80	0.60
1:A:258:ILE:CG2	1:A:261:LEU:HG	2.31	0.60
1:B:570:GLU:HG2	1:B:570:GLU:O	2.00	0.60
1:A:258:ILE:HG12	1:A:303:VAL:HG22	1.84	0.60
1:A:583:ARG:CB	3:A:1101:HOH:O	2.49	0.60
1:B:97:ALA:N	3:B:1105:HOH:O	2.26	0.60
1:B:409:GLN:OE1	1:B:411:TRP:NE1	2.35	0.60
1:A:183:PRO:O	1:A:184:VAL:HG23	2.02	0.60
1:A:174:THR:CG2	1:A:176:PHE:H	2.15	0.59
1:A:420:VAL:HG22	1:A:421:THR:N	2.17	0.59
1:B:136:ILE:HD13	1:B:447:HIS:CB	2.33	0.59
1:A:420:VAL:HG22	1:A:421:THR:H	1.66	0.59
1:B:357:ASN:O	1:B:360:GLN:N	2.26	0.59
1:B:490:GLY:O	1:B:528:PHE:CG	2.53	0.59
1:B:532:ILE:HD12	1:B:532:ILE:N	2.16	0.59
1:B:472:LEU:HA	1:B:579:LEU:O	2.03	0.59
1:A:310:HIS:HD2	1:A:312:VAL:CG2	2.15	0.59
1:A:334:LYS:CE	1:A:345:MET:HG2	2.33	0.59
1:A:431:SER:HB2	1:A:445:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:HG22	1:B:118:ASP:H	1.68	0.59
1:B:543:ILE:HD13	1:B:571:PRO:CD	2.29	0.59
1:A:259:PRO:HG2	1:A:309:LEU:HD12	1.83	0.59
1:B:138:CYS:SG	1:B:139:GLN:N	2.75	0.59
1:B:515:LEU:HD12	1:B:516:GLY:H	1.67	0.59
1:A:24:ALA:O	1:A:27:LEU:N	2.36	0.59
1:A:589:HIS:NE2	3:A:1112:HOH:O	2.32	0.58
1:B:473:LYS:HG3	1:B:579:LEU:CD2	2.29	0.58
1:A:313:HIS:NE2	1:A:419:PRO:HB3	2.17	0.58
1:B:311:THR:CA	1:B:421:THR:CG2	2.58	0.58
1:B:491:ARG:CB	1:B:528:PHE:HD2	2.17	0.58
1:A:269:SER:O	1:A:289:CYS:N	2.37	0.58
1:A:258:ILE:HB	1:A:261:LEU:HG	1.86	0.58
1:A:13:LEU:HD11	1:A:113:MET:HE2	1.85	0.58
1:A:579:LEU:O	1:A:579:LEU:HD12	2.03	0.58
1:A:352:SER:CB	1:A:410:GLN:NE2	2.67	0.57
1:A:174:THR:HG22	1:A:176:PHE:H	1.69	0.57
1:A:122:GLY:HA2	1:A:163:MET:HE2	1.85	0.57
1:A:148:ILE:O	1:A:148:ILE:HG23	2.04	0.57
1:B:148:ILE:N	1:B:185:ALA:HB2	2.19	0.57
1:B:578:SER:O	1:B:590:LYS:HG2	2.05	0.57
1:B:7:ASN:OD1	1:B:8:VAL:N	2.38	0.57
1:A:108:GLN:N	3:A:1107:HOH:O	2.06	0.57
1:A:472:LEU:HG	1:A:474:HIS:NE2	2.19	0.57
1:A:530:ILE:HG22	1:A:531:HIS:O	2.04	0.57
1:A:120:THR:HG21	1:A:150:LEU:HD23	1.87	0.57
1:A:590:LYS:HG3	1:A:591:ARG:N	2.20	0.57
1:B:364:LEU:O	1:B:451:LEU:HD21	2.04	0.57
1:B:485:ASP:HA	1:B:536:LEU:HD12	1.87	0.57
1:A:115:LEU:HD22	1:A:131:LEU:HD13	1.85	0.57
1:A:422:CYS:HB3	1:A:423:PRO:HD2	1.86	0.57
1:B:590:LYS:HG3	1:B:591:ARG:N	2.20	0.57
1:A:290:VAL:HG12	1:A:291:THR:H	1.69	0.56
1:B:140:LYS:HE2	1:B:179:ALA:HA	1.88	0.56
1:B:570:GLU:CD	3:B:1103:HOH:O	2.43	0.56
1:A:113:MET:O	1:A:141:LEU:HA	2.05	0.56
1:A:358:PHE:CE1	1:A:407:PRO:HB3	2.41	0.56
1:A:577:LEU:HD21	1:A:579:LEU:HG	1.87	0.56
1:B:317:ILE:HG21	1:B:428:VAL:HG21	1.86	0.56
1:A:143:VAL:O	1:A:181:ILE:HA	2.06	0.56
1:B:163:MET:O	1:B:166:LYS:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:O	1:B:411:TRP:HB3	2.06	0.56
1:A:257:GLU:HB2	1:A:306:PRO:HA	1.87	0.56
1:A:479:VAL:N	1:A:573:GLN:O	2.32	0.56
1:A:533:PRO:HG2	1:A:534:GLY:H	1.71	0.56
1:A:349:MET:O	1:A:412:ALA:CB	2.53	0.56
1:B:251:SER:HA	1:B:278:THR:O	2.05	0.56
1:B:471:LYS:HE3	1:B:581:PHE:CD2	2.41	0.56
1:B:486:TYR:CD1	1:B:535:GLY:HA2	2.40	0.56
1:A:429:ILE:HG12	1:A:447:HIS:CB	2.36	0.55
1:B:337:ILE:HA	1:B:430:GLY:HA3	1.89	0.55
1:B:475:LYS:HB2	1:B:577:LEU:HD23	1.88	0.55
1:A:430:GLY:O	1:A:431:SER:HB3	2.05	0.55
1:A:141:LEU:HD23	1:A:142:VAL:N	2.21	0.55
1:A:460:ALA:O	1:A:465:PRO:HD3	2.07	0.55
1:B:349:MET:O	1:B:412:ALA:HB1	2.07	0.55
1:A:586:PHE:CD2	1:A:586:PHE:N	2.72	0.55
1:B:510:LEU:HA	1:B:574:HIS:O	2.07	0.55
1:B:325:PHE:CD1	1:B:445:ALA:HA	2.42	0.55
1:A:136:ILE:HD13	1:A:429:ILE:HD11	1.89	0.55
1:A:465:PRO:HA	1:A:584:TYR:CB	2.36	0.55
1:A:317:ILE:CD1	1:A:319:VAL:HG22	2.37	0.55
1:B:117:ILE:HG22	1:B:118:ASP:N	2.22	0.55
1:A:20:LYS:HG3	2:A:1001:GDP:O3B	2.07	0.55
1:B:491:ARG:CB	1:B:528:PHE:CD2	2.90	0.55
1:A:319:VAL:HG21	1:A:412:ALA:CB	2.37	0.54
1:A:368:ASN:O	1:A:370:SER:N	2.40	0.54
1:A:56:PHE:O	1:A:87:GLN:HA	2.07	0.54
1:B:545:THR:CB	1:B:546:PRO:CD	2.85	0.54
1:A:422:CYS:HB3	1:A:423:PRO:CD	2.37	0.54
1:A:334:LYS:HE2	1:A:345:MET:HG2	1.90	0.54
1:B:347:ARG:NH1	1:B:417:GLU:OE2	2.40	0.54
1:A:531:HIS:CG	1:A:532:ILE:H	2.25	0.54
1:B:508:VAL:HG12	1:B:509:HIS:N	2.23	0.54
1:A:135:GLN:HA	1:A:176:PHE:CZ	2.43	0.54
1:A:187:LYS:O	2:A:1001:GDP:C6	2.61	0.54
1:A:335:PHE:CA	1:A:433:LEU:HD23	2.38	0.54
1:B:425:LEU:HA	1:B:450:LEU:O	2.08	0.54
1:B:329:LEU:HD12	1:B:379:TYR:CD2	2.36	0.54
1:A:348:LEU:HD23	1:A:350:PHE:CE1	2.43	0.54
1:B:205:LEU:O	1:B:209:LEU:CB	2.40	0.54
1:B:227:SER:O	1:B:243:GLY:HA3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:SER:O	1:A:31:ALA:HB2	2.08	0.53
1:B:140:LYS:CE	1:B:179:ALA:HA	2.38	0.53
1:B:473:LYS:O	1:B:579:LEU:HG	2.08	0.53
1:B:491:ARG:CA	1:B:528:PHE:CD2	2.91	0.53
1:B:508:VAL:HG12	1:B:509:HIS:H	1.71	0.53
1:B:226:MET:O	1:B:303:VAL:N	2.37	0.53
1:A:140:LYS:HD2	1:A:141:LEU:H	1.73	0.53
1:A:23:LEU:HD23	1:A:27:LEU:HG	1.91	0.53
1:A:250:ILE:CG2	1:A:251:SER:H	2.16	0.53
1:B:479:VAL:HG13	1:B:489:ILE:O	2.07	0.53
1:A:208:LEU:O	1:A:211:SER:N	2.41	0.53
1:B:15:HIS:ND1	1:B:126:GLN:HB3	2.23	0.53
1:B:316:LEU:HD21	1:B:367:PHE:CZ	2.43	0.53
1:A:290:VAL:HG12	1:A:291:THR:N	2.24	0.53
1:A:353:PRO:HG2	1:A:358:PHE:CD1	2.44	0.53
1:B:245:ILE:CD1	1:B:280:ALA:HB3	2.39	0.53
1:A:120:THR:HG21	1:A:150:LEU:CD2	2.39	0.53
1:A:227:SER:HA	3:A:1102:HOH:O	2.09	0.53
1:A:334:LYS:HD2	1:A:347:ARG:HG2	1.91	0.53
1:A:96:HIS:O	1:A:99:LEU:N	2.42	0.53
1:B:477:GLY:N	1:B:575:VAL:O	2.42	0.52
1:A:148:ILE:HG22	1:A:185:ALA:CA	2.39	0.52
1:A:174:THR:HG22	1:A:176:PHE:N	2.24	0.52
1:A:508:VAL:C	1:A:509:HIS:CD2	2.83	0.52
1:A:114:MET:CE	1:A:209:LEU:HD21	2.40	0.52
1:A:257:GLU:OE2	1:A:307:GLU:N	2.40	0.52
1:B:570:GLU:OE1	3:B:1103:HOH:O	2.19	0.52
1:B:148:ILE:HD11	1:B:183:PRO:CB	2.33	0.52
1:B:346:GLY:HA2	1:B:417:GLU:OE1	2.09	0.52
1:A:100:ILE:HG22	1:A:101:ARG:N	2.25	0.52
1:A:319:VAL:HG21	1:A:412:ALA:HB2	1.91	0.52
1:A:101:ARG:CD	1:A:341:HIS:O	2.58	0.52
1:A:274:HIS:O	1:A:276:PRO:HD2	2.09	0.51
1:A:220:PRO:HB3	1:A:281:MET:CG	2.40	0.51
1:B:348:LEU:HD21	1:B:350:PHE:CE1	2.45	0.51
1:B:317:ILE:CG2	1:B:428:VAL:HG21	2.40	0.51
1:B:487:SER:O	1:B:536:LEU:HD21	2.10	0.51
1:A:206:ILE:O	1:A:210:THR:HG23	2.09	0.51
1:A:58:VAL:O	1:A:86:LEU:HB3	2.11	0.51
1:B:322:ILE:HD12	1:B:444:LEU:C	2.31	0.51
1:A:477:GLY:HA2	1:A:492:SER:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:GLY:HA3	1:A:528:PHE:HD2	1.74	0.51
1:A:577:LEU:HD23	1:A:578:SER:N	2.26	0.51
1:B:205:LEU:HG	1:B:209:LEU:HD12	1.93	0.51
1:B:515:LEU:HD12	1:B:516:GLY:N	2.26	0.51
1:A:425:LEU:N	1:A:425:LEU:HD23	2.24	0.51
1:A:589:HIS:CD2	3:A:1112:HOH:O	2.64	0.51
1:B:133:ILE:O	1:B:136:ILE:HB	2.11	0.51
1:B:330:GLN:N	3:B:1104:HOH:O	2.26	0.51
1:A:258:ILE:CD1	1:A:261:LEU:HD21	2.39	0.50
1:A:132:VAL:O	1:A:135:GLN:N	2.43	0.50
1:B:119:VAL:HA	1:B:163:MET:CE	2.41	0.50
1:A:345:MET:O	1:A:417:GLU:HG2	2.11	0.50
1:B:473:LYS:CG	1:B:579:LEU:CD1	2.66	0.50
1:A:220:PRO:HB3	1:A:281:MET:HG2	1.94	0.50
1:A:577:LEU:HD23	1:A:577:LEU:C	2.31	0.50
1:B:9:ASN:HB2	1:B:109:ILE:O	2.11	0.49
1:A:346:GLY:HA2	1:A:416:PHE:HA	1.94	0.49
1:A:433:LEU:O	1:A:433:LEU:CD1	2.46	0.49
1:B:579:LEU:C	1:B:579:LEU:HD12	2.33	0.49
1:A:13:LEU:HD11	1:A:113:MET:HE3	1.92	0.49
1:A:341:HIS:N	3:A:1114:HOH:O	2.45	0.49
1:A:585:VAL:CG2	1:A:586:PHE:N	2.76	0.49
1:A:320:GLU:O	1:A:446:PHE:HB2	2.12	0.49
1:B:329:LEU:HA	3:B:1104:HOH:O	2.12	0.49
1:B:490:GLY:C	1:B:528:PHE:HD2	2.06	0.49
1:B:585:VAL:CG2	1:B:586:PHE:N	2.76	0.49
1:A:103:ILE:HD12	1:A:113:MET:HE1	1.93	0.49
1:A:334:LYS:HE3	1:A:345:MET:HG2	1.94	0.48
1:A:490:GLY:H	1:A:528:PHE:HB3	1.77	0.48
1:A:508:VAL:C	1:A:509:HIS:HD2	2.15	0.48
1:A:531:HIS:CG	1:A:532:ILE:N	2.81	0.48
1:B:311:THR:CB	1:B:421:THR:HG21	2.39	0.48
1:B:485:ASP:C	1:B:536:LEU:HG	2.33	0.48
1:A:338:THR:N	1:A:429:ILE:O	2.32	0.48
1:B:329:LEU:HB2	1:B:379:TYR:HB3	1.93	0.48
1:B:422:CYS:HB2	1:B:423:PRO:CD	2.44	0.48
1:B:471:LYS:CB	1:B:581:PHE:HB3	2.43	0.48
1:A:433:LEU:HD12	1:A:433:LEU:C	2.31	0.48
1:A:272:MET:HB3	1:A:286:LEU:CB	2.44	0.48
1:B:519:ASP:O	1:B:520:SER:CB	2.61	0.48
1:A:466:ARG:HG3	1:B:505:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:O	1:B:378:GLN:HA	2.14	0.48
1:A:217:THR:C	1:A:218:ARG:HG2	2.34	0.48
1:A:582:LYS:HB2	1:A:585:VAL:HG12	1.95	0.48
1:B:117:ILE:HG23	1:B:123:MET:HA	1.95	0.48
1:A:164:THR:O	1:A:168:GLN:HG3	2.14	0.47
1:A:335:PHE:HA	1:A:433:LEU:HD23	1.96	0.47
1:B:311:THR:HA	1:B:421:THR:CB	2.44	0.47
1:B:590:LYS:HG3	1:B:591:ARG:H	1.79	0.47
1:A:313:HIS:ND1	1:A:457:ARG:HA	2.29	0.47
1:B:373:TYR:N	1:B:468:LYS:O	2.42	0.47
1:A:114:MET:HE2	1:A:209:LEU:HD21	1.97	0.47
1:A:329:LEU:HB2	1:A:379:TYR:HB3	1.97	0.47
1:A:5:ARG:NH1	1:A:272:MET:O	2.48	0.47
1:B:372:GLU:HG2	1:B:468:LYS:CB	2.45	0.47
1:B:469:VAL:O	1:B:582:LYS:HA	2.13	0.47
1:A:100:ILE:O	1:A:103:ILE:HG22	2.14	0.47
1:A:351:PHE:CZ	1:A:411:TRP:HB2	2.48	0.47
1:B:317:ILE:HD12	1:B:317:ILE:O	2.14	0.47
1:A:318:SER:O	1:A:448:GLY:HA3	2.15	0.47
1:A:334:LYS:HD2	1:A:347:ARG:CG	2.45	0.47
1:A:568:ARG:O	1:A:569:SER:OG	2.24	0.47
1:A:259:PRO:HD2	3:A:1109:HOH:O	2.15	0.47
1:A:93:CYS:CB	1:A:94:PRO:HD2	2.45	0.47
1:A:153[B]:GLU:CD	3:A:1103:HOH:O	2.46	0.47
1:A:9:ASN:HD21	1:A:244:THR:HG21	1.80	0.47
1:B:528:PHE:O	1:B:529:LYS:CB	2.60	0.47
1:B:245:ILE:HB	1:B:281:MET:O	2.15	0.47
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.60	0.46
1:A:225:LEU:HD11	1:A:302:LEU:CD2	2.41	0.46
1:A:224:PHE:CG	1:A:250:ILE:HD11	2.49	0.46
1:A:99:LEU:O	1:A:103:ILE:HG22	2.14	0.46
1:B:132:VAL:O	1:B:136:ILE:HG13	2.16	0.46
1:B:347:ARG:HG2	3:B:1106:HOH:O	2.15	0.46
1:B:202:ILE:CB	1:B:203:PRO:HD3	2.45	0.46
1:B:338:THR:HA	1:B:343:THR:HA	1.96	0.46
1:B:580:THR:HG23	1:B:590:LYS:HD2	1.88	0.46
1:B:346:GLY:O	1:B:347:ARG:HD3	2.16	0.46
1:A:466:ARG:NH1	1:B:589:HIS:ND1	2.64	0.46
1:A:477:GLY:HA3	1:A:492:SER:OG	2.15	0.46
1:A:258:ILE:CB	1:A:261:LEU:HG	2.44	0.46
1:B:348:LEU:HG	1:B:349:MET:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:CG2	1:B:88:VAL:HG22	2.45	0.46
1:B:316:LEU:HD12	1:B:412:ALA:O	2.16	0.46
1:B:477:GLY:HA3	1:B:492:SER:CB	2.30	0.46
1:B:8:VAL:HG23	1:B:88:VAL:HG13	1.96	0.46
1:A:485:ASP:O	1:A:536:LEU:N	2.49	0.46
1:B:347:ARG:O	1:B:348:LEU:HB2	2.16	0.46
1:A:13:LEU:HD11	1:A:113:MET:HB3	1.98	0.46
1:A:115:LEU:HB2	1:A:141:LEU:HD21	1.98	0.46
1:A:267:VAL:O	1:A:267:VAL:HG12	2.15	0.46
1:A:132:VAL:HG13	1:A:133:ILE:H	1.81	0.46
1:A:352:SER:CB	1:A:410:GLN:HE21	2.27	0.46
1:A:313:HIS:HE2	1:A:419:PRO:HB3	1.78	0.46
1:A:480:GLU:HG3	1:A:481:ARG:N	2.27	0.46
1:A:413:LEU:HD23	1:A:415:GLU:HG3	1.97	0.46
1:B:473:LYS:H	1:B:579:LEU:CD1	2.29	0.46
1:A:353:PRO:HG2	1:A:358:PHE:HD1	1.80	0.45
1:B:582:LYS:HB2	1:B:585:VAL:HG12	1.98	0.45
1:A:251:SER:N	1:A:254:ASP:OD2	2.49	0.45
1:A:590:LYS:HG3	1:A:591:ARG:H	1.79	0.45
1:B:187:LYS:O	2:B:1001:GDP:C5	2.66	0.45
1:B:417:GLU:HG3	3:B:1106:HOH:O	2.16	0.45
1:A:339:VAL:O	1:A:427:LEU:O	2.35	0.45
1:B:275:MET:N	1:B:276:PRO:CD	2.77	0.45
1:B:136:ILE:CD1	1:B:447:HIS:HB3	2.41	0.45
1:A:114:MET:HE2	1:A:209:LEU:CD2	2.47	0.45
1:A:258:ILE:HB	1:A:261:LEU:CG	2.46	0.45
1:A:180:PRO:HG2	1:A:208:LEU:HD21	1.99	0.45
1:A:21:THR:HG22	1:A:21:THR:O	2.16	0.45
1:A:493:LEU:O	1:A:494:PHE:C	2.54	0.45
1:B:208:LEU:O	1:B:211:SER:CB	2.65	0.45
1:B:494:PHE:O	1:B:495:LYS:CB	2.64	0.45
1:A:113:MET:HB2	1:A:141:LEU:CD1	2.46	0.45
1:B:20:LYS:CA	2:B:1001:GDP:O1A	2.61	0.44
1:B:203:PRO:O	1:B:204:GLU:C	2.55	0.44
1:B:322:ILE:HG13	1:B:446:PHE:CA	2.45	0.44
1:A:140:LYS:CD	1:A:141:LEU:H	2.31	0.44
1:A:431:SER:CB	1:A:445:ALA:HB3	2.46	0.44
1:B:372:GLU:CG	1:B:582:LYS:HZ2	2.28	0.44
1:A:202:ILE:HB	1:A:203:PRO:HD3	2.00	0.44
1:B:411:TRP:O	1:B:412:ALA:HB2	2.17	0.44
1:B:318:SER:HA	1:B:411:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ARG:HD2	1:B:486:TYR:CE2	2.53	0.44
1:B:590:LYS:CG	1:B:591:ARG:N	2.81	0.44
1:A:261:LEU:HD12	1:A:261:LEU:C	2.38	0.44
1:A:258:ILE:HG22	1:A:261:LEU:HG	2.00	0.44
1:A:256:VAL:O	1:A:264:VAL:HA	2.18	0.44
1:A:338:THR:HA	1:A:343:THR:HA	1.99	0.44
1:A:423:PRO:HB2	1:A:426:CYS:HB3	1.99	0.44
1:A:7:ASN:HD21	1:A:89:THR:CG2	2.31	0.44
1:A:224:PHE:CZ	1:A:226:MET:HB2	2.53	0.44
1:A:431:SER:CB	1:A:445:ALA:H	2.30	0.44
1:A:590:LYS:CG	1:A:591:ARG:N	2.81	0.44
1:B:148:ILE:HB	1:B:185:ALA:HB2	2.00	0.44
1:B:527:LYS:O	1:B:528:PHE:HB2	2.17	0.44
1:A:319:VAL:HG12	1:A:320:GLU:N	2.33	0.44
1:A:334:LYS:HB3	1:A:433:LEU:HD21	1.99	0.44
1:A:588:THR:HG23	1:A:589:HIS:N	2.13	0.44
1:B:425:LEU:HD23	1:B:425:LEU:N	2.32	0.44
1:A:144:VAL:HG11	1:A:205:LEU:HD13	2.00	0.43
1:A:142:VAL:HG22	1:A:180:PRO:HG2	1.99	0.43
1:B:579:LEU:HA	1:B:590:LYS:HB2	2.00	0.43
1:A:323:PRO:O	1:A:325:PHE:N	2.51	0.43
1:A:332:LYS:O	1:A:347:ARG:NH1	2.52	0.43
1:A:101:ARG:HG3	1:A:341:HIS:C	2.39	0.43
1:B:584:TYR:C	1:B:585:VAL:O	2.51	0.43
1:B:212:GLN:C	1:B:214:SER:H	2.22	0.43
1:A:322:ILE:HG23	1:A:323:PRO:HD2	2.00	0.43
1:B:166:LYS:HG2	1:B:167:MET:N	2.33	0.43
1:B:224:PHE:HD2	1:B:304:CYS:CA	2.28	0.43
1:A:100:ILE:HA	1:A:103:ILE:HG22	2.01	0.43
1:B:245:ILE:HD12	1:B:280:ALA:CB	2.48	0.43
1:B:316:LEU:CD2	1:B:367:PHE:CE2	3.02	0.43
1:A:420:VAL:CG2	1:A:421:THR:H	2.30	0.43
1:A:477:GLY:HA2	1:A:492:SER:HB3	2.01	0.43
1:A:113:MET:HG2	1:A:138:CYS:CB	2.49	0.43
1:A:317:ILE:HA	1:A:449:ILE:O	2.18	0.43
1:A:7:ASN:OD1	1:A:8:VAL:N	2.51	0.43
1:B:584:TYR:O	1:B:585:VAL:C	2.56	0.43
1:A:339:VAL:HG12	1:A:426:CYS:SG	2.58	0.43
1:A:317:ILE:HG23	1:A:414:VAL:CG2	2.48	0.43
1:B:26:ALA:O	1:B:30:THR:N	2.50	0.43
1:B:317:ILE:HD12	1:B:317:ILE:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LEU:HD12	1:B:502:LEU:N	2.34	0.43
1:A:377:GLU:HG3	1:A:377:GLU:O	2.19	0.43
1:A:12:VAL:O	1:A:99:LEU:HD11	2.19	0.43
1:B:220:PRO:CB	1:B:249:SER:HB2	2.47	0.43
1:B:545:THR:CB	1:B:546:PRO:HD2	2.49	0.43
1:A:319:VAL:CG2	1:A:412:ALA:HB3	2.49	0.42
1:B:347:ARG:CZ	1:B:417:GLU:OE2	2.67	0.42
1:A:116:VAL:O	1:A:117:ILE:HD13	2.19	0.42
1:A:117:ILE:HG23	1:A:122:GLY:O	2.17	0.42
1:A:406:CYS:CB	1:A:407:PRO:CD	2.97	0.42
1:A:466:ARG:HD2	1:B:589:HIS:CE1	2.54	0.42
1:B:450:LEU:HD23	1:B:452:HIS:N	2.34	0.42
1:B:484:ASP:O	1:B:536:LEU:HD11	2.20	0.42
1:B:568:ARG:O	1:B:569:SER:CB	2.66	0.42
1:B:580:THR:OG1	1:B:589:HIS:O	2.30	0.42
1:A:360:GLN:HG2	1:A:361:GLU:N	2.34	0.42
1:B:362:PRO:HA	1:B:409:GLN:HE21	1.78	0.42
1:B:447:HIS:O	1:B:447:HIS:ND1	2.52	0.42
1:B:473:LYS:H	1:B:579:LEU:HD12	1.84	0.42
1:B:119:VAL:HA	1:B:163:MET:HE1	2.01	0.42
1:B:337:ILE:HA	1:B:430:GLY:CA	2.49	0.42
1:A:323:PRO:C	1:A:325:PHE:H	2.23	0.42
1:A:420:VAL:CG2	1:A:421:THR:N	2.82	0.42
1:A:220:PRO:HD3	1:A:281:MET:CE	2.48	0.42
1:A:466:ARG:HD3	1:A:466:ARG:HA	1.92	0.42
1:A:466:ARG:CD	1:B:589:HIS:HE1	2.32	0.42
1:A:140:LYS:CG	1:A:141:LEU:H	2.33	0.42
1:A:250:ILE:HG23	1:A:250:ILE:HD12	1.76	0.42
1:B:322:ILE:HD12	1:B:445:ALA:N	2.34	0.42
1:A:144:VAL:HG12	1:A:182:ILE:CB	2.39	0.42
1:A:368:ASN:O	1:A:371:GLN:HG2	2.19	0.42
1:A:579:LEU:HA	1:A:590:LYS:CB	2.39	0.42
1:A:149:ASP:OD1	1:A:150:LEU:HD13	2.20	0.42
1:B:587:ASP:O	1:B:588:THR:HB	2.20	0.42
1:B:245:ILE:HD12	1:B:280:ALA:HB3	2.02	0.41
1:A:114:MET:HA	1:A:142:VAL:O	2.19	0.41
1:A:422:CYS:CB	1:A:423:PRO:CD	2.97	0.41
1:B:471:LYS:HB2	1:B:581:PHE:HB3	2.02	0.41
1:A:140:LYS:HD2	1:A:141:LEU:N	2.36	0.41
1:A:185:ALA:HB3	1:A:200:GLN:OE1	2.20	0.41
1:A:466:ARG:HH11	1:B:589:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:PHE:CE2	1:B:304:CYS:HA	2.55	0.41
1:B:364:LEU:C	1:B:451:LEU:HD21	2.40	0.41
1:A:147:LYS:C	1:A:149:ASP:H	2.24	0.41
1:B:486:TYR:HB3	1:B:532:ILE:O	2.20	0.41
1:A:469:VAL:O	1:A:582:LYS:HA	2.20	0.41
1:A:490:GLY:CA	1:A:528:PHE:HD2	2.33	0.41
1:B:313:HIS:CD2	1:B:419:PRO:HB3	2.55	0.41
1:B:346:GLY:O	1:B:347:ARG:NH1	2.49	0.41
1:B:475:LYS:HB3	1:B:493:LEU:CB	2.50	0.41
1:A:220:PRO:CG	1:A:281:MET:HE2	2.45	0.41
1:A:19:GLY:HA3	1:A:146:ASN:ND2	2.36	0.41
1:A:590:LYS:CG	1:A:591:ARG:H	2.34	0.41
1:B:590:LYS:O	1:B:591:ARG:CB	2.69	0.41
1:A:23:LEU:HD23	1:A:23:LEU:C	2.40	0.41
1:A:312:VAL:HG13	1:A:314:ALA:O	2.21	0.41
1:B:529:LYS:O	1:B:530:ILE:HD12	2.21	0.41
1:A:149:ASP:OD1	1:A:150:LEU:CD1	2.69	0.41
1:B:187:LYS:C	2:B:1001:GDP:C6	2.90	0.41
1:B:335:PHE:CE2	1:B:446:PHE:HE2	2.39	0.41
1:A:344:VAL:HG11	1:A:420:VAL:HB	2.03	0.41
1:A:451:LEU:O	1:A:452:HIS:HB2	2.20	0.41
1:B:528:PHE:HD1	1:B:529:LYS:H	1.67	0.41
1:A:240:VAL:HG12	1:A:241:MET:N	2.36	0.40
1:A:590:LYS:O	1:A:591:ARG:CB	2.69	0.40
1:A:272:MET:O	1:A:272:MET:HG3	2.21	0.40
1:A:357:ASN:ND2	1:A:360:GLN:OE1	2.54	0.40
1:A:418:LYS:O	1:A:420:VAL:N	2.54	0.40
1:B:318:SER:HA	1:B:411:TRP:HD1	1.86	0.40
1:A:528:PHE:HD1	1:A:528:PHE:HA	1.66	0.40
1:A:511:SER:CB	1:A:574:HIS:CB	2.99	0.40
1:A:86:LEU:HD12	1:A:87:GLN:N	2.36	0.40
1:A:492:SER:O	1:A:493:LEU:CB	2.69	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	459/616 (74%)	340 (74%)	99 (22%)	20 (4%)	3 23
1	B	428/616 (70%)	330 (77%)	82 (19%)	16 (4%)	4 28
All	All	887/1232 (72%)	670 (76%)	181 (20%)	36 (4%)	3 26

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	ILE
1	A	275	MET
1	A	277	ILE
1	A	324	TYR
1	A	369	PHE
1	B	166	LYS
1	A	31	ALA
1	A	119	VAL
1	A	291	THR
1	B	23	LEU
1	B	545	THR
1	A	148	ILE
1	A	216	PRO
1	A	493	LEU
1	A	533	PRO
1	B	100	ILE
1	B	527	LYS
1	B	533	PRO
1	B	572	SER
1	A	24	ALA
1	B	202	ILE
1	B	277	ILE
1	B	472	LEU
1	B	491	ARG
1	A	191	PRO
1	A	571	PRO
1	B	571	PRO
1	A	61	PRO
1	A	104	ILE
1	B	148	ILE
1	B	213	ILE

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Mol	Chain	Res	Type
1	A	263	VAL
1	A	518	ILE
1	A	419	PRO
1	B	488	VAL
1	B	543	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	261/524 (50%)	251 (96%)	10 (4%)	40 76
1	B	160/524 (30%)	156 (98%)	4 (2%)	55 84
All	All	421/1048 (40%)	407 (97%)	14 (3%)	45 79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	THR
1	A	218	ARG
1	A	228	VAL
1	A	274	HIS
1	A	348	LEU
1	A	358	PHE
1	A	421	THR
1	A	528	PHE
1	A	529	LYS
1	A	586	PHE
1	B	135	GLN
1	B	324	TYR
1	B	528	PHE
1	B	584	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	310	HIS
1	A	341	HIS
1	A	410	GLN
1	A	509	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

2 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	GDP	A	1001	-	24,30,30	1.62	5 (20%)	26,47,47	1.96	4 (15%)
2	GDP	B	1001	-	24,30,30	1.62	6 (25%)	26,47,47	1.98	5 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	A	1001	-	-	0/12/32/32	0/3/3/3
2	GDP	B	1001	-	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GDP	C6-C5	-3.76	1.33	1.41
2	B	1001	GDP	C6-C5	-3.76	1.33	1.41
2	A	1001	GDP	C5-C4	-2.93	1.33	1.40
2	B	1001	GDP	C5-C4	-2.93	1.33	1.40
2	B	1001	GDP	PB-O2B	-2.15	1.47	1.54
2	A	1001	GDP	PB-O2B	-2.14	1.47	1.54
2	B	1001	GDP	PB-O3B	-2.14	1.47	1.54
2	A	1001	GDP	C2-N1	2.38	1.39	1.35
2	B	1001	GDP	C2-N1	2.39	1.39	1.35
2	B	1001	GDP	C6-N1	3.91	1.40	1.33
2	A	1001	GDP	C6-N1	3.95	1.40	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	GDP	N3-C2-N1	-6.08	119.28	127.56
2	A	1001	GDP	N3-C2-N1	-6.01	119.38	127.56
2	A	1001	GDP	C4'-O4'-C1'	-5.35	103.97	109.64
2	B	1001	GDP	C4'-O4'-C1'	-5.32	104.00	109.64
2	A	1001	GDP	C5-C6-N1	-2.96	119.66	123.52
2	B	1001	GDP	C5-C6-N1	-2.94	119.68	123.52
2	A	1001	GDP	C6-N1-C2	2.00	118.23	115.88
2	B	1001	GDP	C6-N1-C2	2.04	118.28	115.88
2	B	1001	GDP	O3B-PB-O2B	2.40	116.25	107.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GDP	4	0
2	B	1001	GDP	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	480/616 (77%)	-0.54	1 (0%) 95 94	27, 69, 101, 114	0
1	B	451/616 (73%)	-0.26	16 (3%) 48 38	44, 95, 149, 168	0
All	All	931/1232 (75%)	-0.40	17 (1%) 71 62	27, 81, 129, 168	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	VAL	5.5
1	B	268	LYS	5.0
1	B	299	GLU	4.9
1	B	287	GLY	4.5
1	B	269	SER	4.1
1	B	288	ILE	3.9
1	B	298	LEU	3.7
1	B	292	GLN	3.3
1	B	117	ILE	2.9
1	B	251	SER	2.8
1	B	286	LEU	2.5
1	A	442	CYS	2.3
1	B	271	GLN	2.3
1	B	242	THR	2.2
1	B	293	PHE	2.2
1	B	263	VAL	2.1
1	B	278	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GDP	A	1001	28/28	0.89	0.17	0.04	72,93,113,129	0
2	GDP	B	1001	28/28	0.80	0.18	-0.06	122,135,153,158	0

6.5 Other polymers (i)

There are no such residues in this entry.