Full wwPDB X-ray Structure Validation Report (i)

Sep 24, 2023 – 12:51 PM EDT

PDB ID	:	5UJB
Title	:	Structure of a Mcl-1 Inhibitor Binding to Site 3 of Human Serum Albumin
Authors	:	Zhao, B.
Deposited on	:	2017-01-17
Resolution	:	2.70 Å(reported)

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

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

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

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

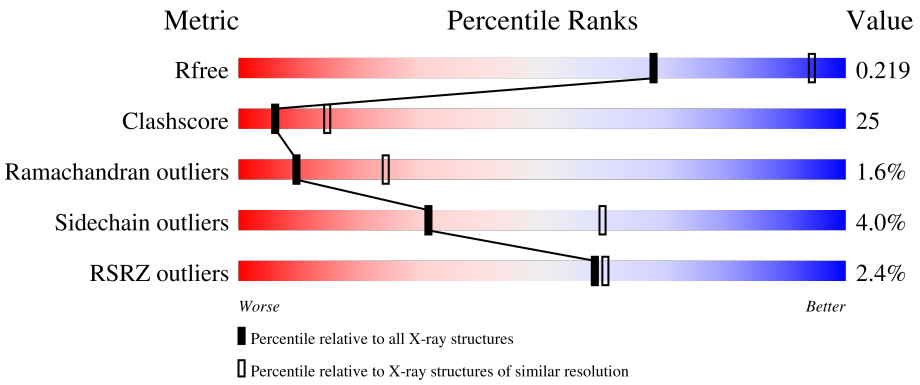
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	609	2% 54% 36% • 7%
1	B	609	2% 52% 38% • 7%

2 Entry composition (i)

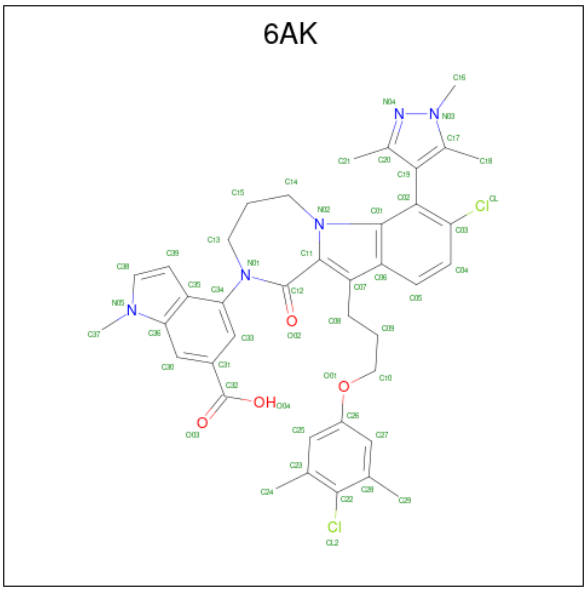
There are 3 unique types of molecules in this entry. The entry contains 8812 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Serum albumin.

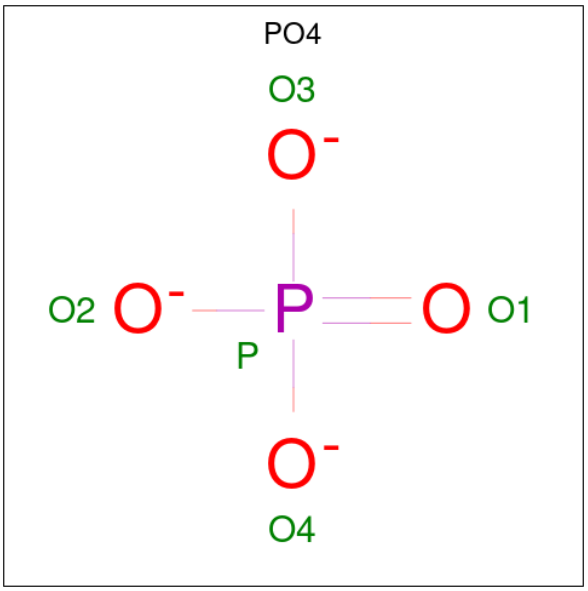
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	568	4364	2760	736	828	40	0	0	0
1	B	565	4338	2749	722	826	41	0	0	0

- Molecule 2 is 4-{8-chloro-11-[3-(4-chloro-3,5-dimethylphenoxy)propyl]-1-oxo-7-(1,3,5-trimethyl-1H-pyrazol-4-yl)-4,5-dihydro-1H-[1,4]diazepino[1,2-a]indol-2(3H)-yl}-1-methyl-1H-indole-6-carboxylic acid (three-letter code: 6AK) (formula: $C_{39}H_{39}Cl_2N_5O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	50	39	2	5	4	0	0
2	B	1	50	39	2	5	4	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



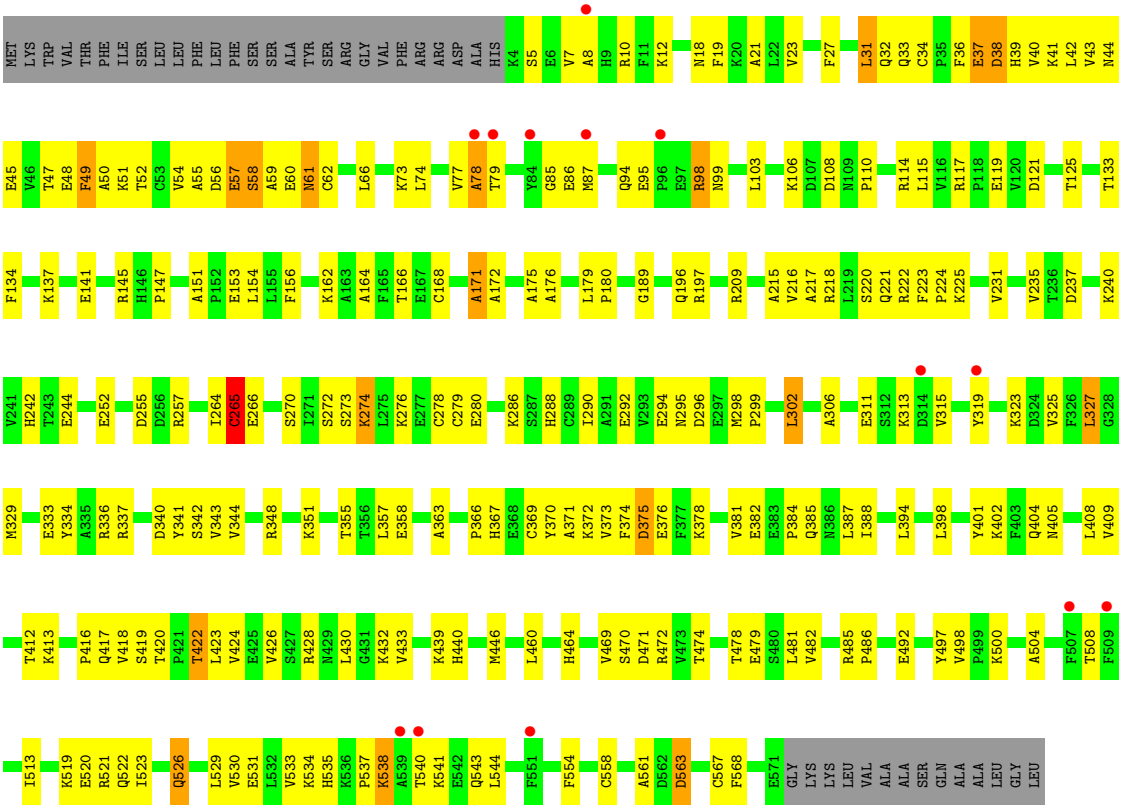
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

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

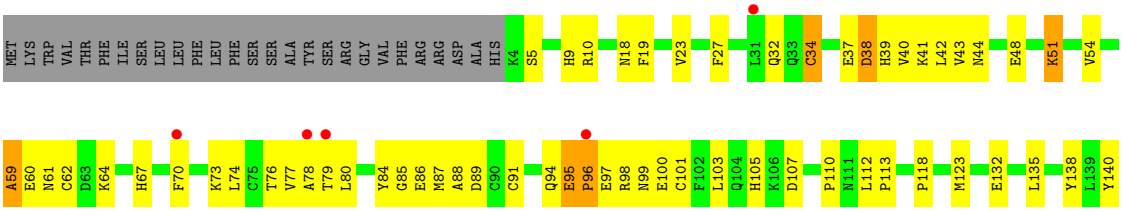
• Molecule 1: Serum albumin

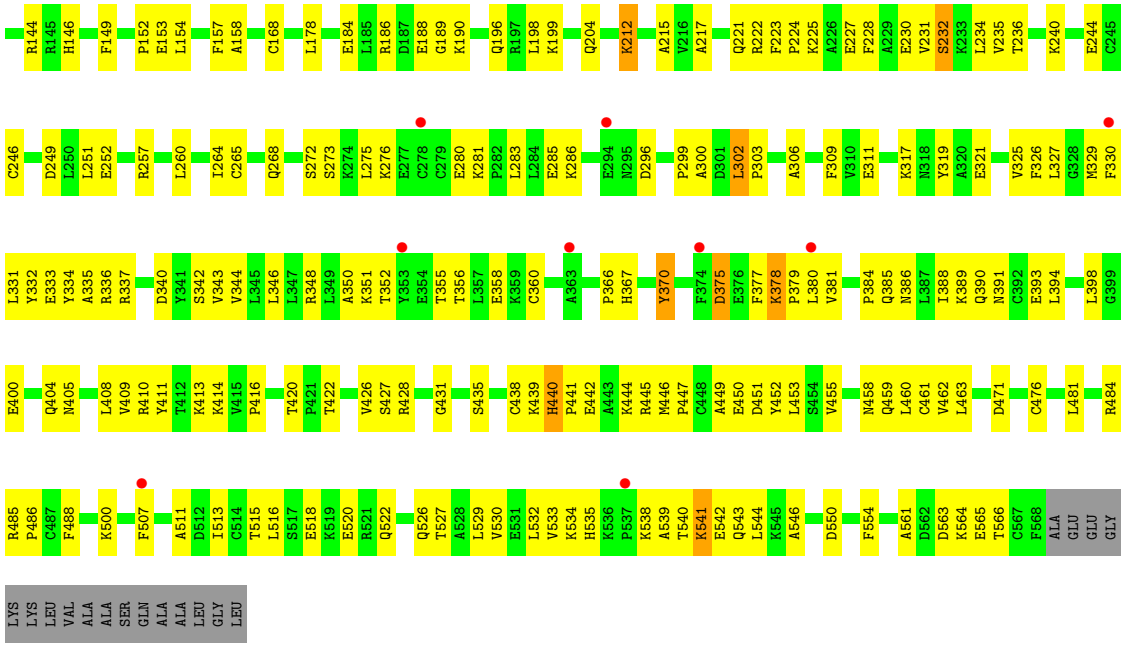
Chain A:



• Molecule 1: Serum albumin

Chain B:




R144 R145 H146 F149 P152 E153 L154 F157 A158 C168 L178 E184 L185 R186 D187 E188 G189 K190 Q196 R197 L198 K199 Q204 K212 A215 V216 A217 Q221 R222 F223 P224 K225 A226 E227 F228 A229 E230 V231 S232 K233 L234 V235 T236 K240 E244 C245
C246 D249 L250 L251 E252 R257 L260 I264 C265 Q268 S272 S273 K274 L275 K276 E277 C278 C279 E280 K281 P282 L283 L284 E285 K286 E294 N295 D296 P299 A300 D301 L302 P303 A306 F309 V310 E311 K317 N318 Y319 A320 E321 V325 F326 L327 G328 M329 F330
L331 Y332 E333 Y334 A335 R336 R337 D340 Y341 S342 V343 V344 L345 L346 L347 R348 L349 A350 K351 T352 Y353 E354 T355 T356 L357 E358 K359 C360 A363 P366 H367 Y370 F374 D375 E376 F377 K378 P379 L380 V381 P384 Q385 N386 L387 I388 K389 Q390 N391 C392 E393 L394 L398 G399
E400 Q404 N405 L408 V409 R410 Y411 T412 K413 K414 V415 P416 T420 P421 T422 V426 S427 R428 G431 S435 C438 K439 H440 P441 E442 A443 K444 R445 M446 P447 C448 A449 E450 D451 Y452 L453 S454 V455 N458 Q459 L460 C461 V462 L463 D471 C476 L481 R484
R485 P486 C487 F488 K500 F507 A511 D512 I513 C514 T515 L516 S517 E518 K519 E520 R521 Q522 Q526 T527 A528 L529 V530 E531 L532 V533 K534 H535 K536 P537 K538 A539 T540 K541 E542 Q543 L544 K545 A546 D550 F554 A561 D562 D563 K564 E565 T566 C567 F568 ALA GLU GLU GLY
LYS LYS LEU VAL ALA ALA SER GLN ALA ALA LEU GLY LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.84Å 182.34Å 58.92Å 90.00° 105.15° 90.00°	Depositor
Resolution (Å)	28.76 – 2.70 48.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.9 (28.76-2.70) 92.4 (48.26-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.174 , 0.215 0.186 , 0.219	Depositor DCC
R_{free} test set	2003 reflections (6.55%)	wwPDB-VP
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.299 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8812	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 6AK

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	0.56	0/4448	0.80	3/6024 (0.0%)
1	B	0.57	1/4425 (0.0%)	0.78	1/6001 (0.0%)
All	All	0.56	1/8873 (0.0%)	0.79	4/12025 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	476	CYS	CB-SG	5.09	1.90	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	66	LEU	CA-CB-CG	6.53	130.31	115.30
1	A	567	CYS	CA-CB-SG	6.33	125.40	114.00
1	A	327	LEU	CB-CG-CD2	-5.68	101.34	111.00
1	B	375	ASP	C-N-CA	-5.14	108.86	121.70

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	4364	0	4111	215	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4338	0	4082	208	0
2	A	50	0	0	4	0
2	B	50	0	0	4	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
All	All	8812	0	8193	421	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 25.

All (421) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ALA:HB3	1:A:62:CYS:SG	1.46	1.55
1:A:302:LEU:HD12	1:A:337:ARG:NH1	1.27	1.48
1:A:302:LEU:CD1	1:A:337:ARG:HH12	1.38	1.35
1:A:59:ALA:CB	1:A:62:CYS:SG	2.20	1.28
1:A:265:CYS:SG	1:A:279:CYS:SG	1.45	1.23
1:A:265:CYS:SG	1:A:279:CYS:CB	2.39	1.10
1:A:540:THR:HB	1:A:544:LEU:HD11	1.37	1.01
1:A:302:LEU:CD1	1:A:337:ARG:NH1	2.10	0.97
1:B:408:LEU:HD23	1:B:427:SER:CB	1.94	0.97
1:A:57:GLU:O	1:A:59:ALA:N	1.98	0.96
1:B:438:CYS:O	1:B:440:HIS:N	2.02	0.92
1:B:408:LEU:HD23	1:B:427:SER:HB3	1.49	0.91
1:B:51:LYS:HA	1:B:54:VAL:HG12	1.54	0.89
1:B:95:GLU:O	1:B:97:GLU:N	2.08	0.86
1:A:302:LEU:HD12	1:A:337:ARG:CZ	2.06	0.86
1:A:540:THR:CB	1:A:544:LEU:HD11	2.04	0.86
1:A:274:LYS:NZ	1:A:294:GLU:OE1	2.11	0.84
1:A:367:HIS:HA	1:A:370:TYR:CE1	2.13	0.84
1:A:412:THR:HG22	1:A:423:LEU:HD13	1.58	0.84
1:A:319:TYR:OH	1:A:358:GLU:OE1	1.97	0.82
1:A:42:LEU:HD22	1:A:73:LYS:HG3	1.59	0.81
1:B:204:GLN:NE2	1:B:246:CYS:HB3	1.95	0.81
1:A:216:VAL:O	1:A:220:SER:OG	1.98	0.81
1:A:531:GLU:O	1:A:535:HIS:ND1	2.13	0.81
1:B:377:PHE:O	1:B:380:LEU:HB2	1.81	0.81
1:B:96:PRO:O	1:B:97:GLU:HG3	1.82	0.80
1:A:114:ARG:H	1:A:114:ARG:HD2	1.44	0.80
1:B:408:LEU:CD2	1:B:427:SER:HB2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:N	1:B:84:TYR:OH	2.15	0.79
1:B:228:PHE:O	1:B:232:SER:OG	1.99	0.79
1:A:540:THR:CA	1:A:544:LEU:HD11	2.14	0.78
1:B:408:LEU:CD2	1:B:427:SER:CB	2.62	0.78
1:B:414:LYS:NZ	1:B:488:PHE:O	2.17	0.77
1:B:67:HIS:CD2	1:B:99:ASN:HD22	2.02	0.77
1:B:408:LEU:HD11	1:B:526:GLN:HB3	1.66	0.77
1:B:204:GLN:HE22	1:B:246:CYS:HB3	1.49	0.76
1:B:34:CYS:HB3	1:B:39:HIS:CE1	2.21	0.75
1:B:300:ALA:O	1:B:302:LEU:HD12	1.86	0.75
1:B:152:PRO:HB2	1:B:257:ARG:HH11	1.52	0.74
1:A:10:ARG:NH1	1:A:255:ASP:OD2	2.21	0.74
1:A:162:LYS:O	1:A:166:THR:HG23	1.88	0.74
1:B:67:HIS:NE2	1:B:249:ASP:OD1	2.22	0.72
1:A:540:THR:HA	1:A:544:LEU:CD1	2.19	0.72
1:B:408:LEU:CD1	1:B:526:GLN:HB3	2.20	0.72
1:B:67:HIS:CG	1:B:99:ASN:ND2	2.58	0.71
1:A:323:LYS:O	1:A:327:LEU:HD12	1.90	0.71
1:A:432:LYS:NZ	3:A:801:PO4:O2	2.20	0.71
1:A:513:ILE:O	1:A:521:ARG:NH1	2.23	0.71
1:A:40:VAL:O	1:A:44:ASN:ND2	2.22	0.71
1:B:352:THR:O	1:B:355:THR:OG1	2.09	0.71
1:A:222:ARG:HG2	1:A:223:PHE:CE1	2.26	0.71
1:B:306:ALA:O	1:B:311:GLU:HG3	1.90	0.71
1:A:59:ALA:HB2	1:A:62:CYS:SG	2.26	0.70
1:B:260:LEU:O	1:B:264:ILE:HG13	1.90	0.70
1:B:352:THR:HG21	1:B:380:LEU:HD11	1.71	0.70
1:A:344:VAL:HG22	1:A:348:ARG:HH12	1.56	0.70
1:A:302:LEU:HB3	1:A:337:ARG:NH1	2.07	0.70
1:A:36:PHE:O	1:A:40:VAL:HG23	1.92	0.70
1:B:224:PRO:HD2	1:B:296:ASP:HB3	1.73	0.70
1:B:232:SER:O	1:B:236:THR:OG1	2.10	0.69
1:B:231:VAL:O	1:B:235:VAL:HG12	1.91	0.69
1:B:32:GLN:HE22	1:B:107:ASP:H	1.39	0.69
1:B:317:LYS:O	1:B:321:GLU:HB2	1.91	0.69
1:A:98:ARG:HG3	1:A:99:ASN:N	2.08	0.68
1:A:540:THR:HA	1:A:544:LEU:HD11	1.73	0.68
1:A:77:VAL:O	1:A:79:THR:N	2.26	0.68
1:A:216:VAL:HG12	1:A:235:VAL:HG21	1.75	0.68
1:A:439:LYS:HE2	1:A:440:HIS:CE1	2.29	0.68
1:A:114:ARG:HD2	1:A:114:ARG:N	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:THR:O	1:A:478:THR:HG23	1.93	0.67
1:B:342:SER:O	1:B:346:LEU:HD12	1.93	0.67
1:B:386:ASN:OD1	1:B:390:GLN:NE2	2.28	0.67
1:B:461:CYS:SG	1:B:484:ARG:NH1	2.67	0.67
1:A:439:LYS:HE2	1:A:440:HIS:NE2	2.10	0.66
1:B:539:ALA:HB1	1:B:543:GLN:HE21	1.61	0.66
1:A:540:THR:CA	1:A:544:LEU:CD1	2.74	0.66
1:A:272:SER:OG	1:A:273:SER:N	2.27	0.66
1:B:522:GLN:O	1:B:526:GLN:HG3	1.96	0.66
1:B:283:LEU:HA	1:B:286:LYS:HB2	1.78	0.65
1:B:273:SER:OG	1:B:296:ASP:OD1	2.14	0.65
1:A:366:PRO:CB	1:A:370:TYR:CE2	2.80	0.65
1:A:313:LYS:NZ	1:A:367:HIS:H	1.95	0.64
1:A:561:ALA:C	1:A:563:ASP:H	2.00	0.64
1:A:59:ALA:O	1:A:60:GLU:HB3	1.97	0.64
1:A:215:ALA:HB3	1:A:235:VAL:HG13	1.79	0.64
1:B:138:TYR:HA	2:B:802:6AK:C04	2.27	0.64
1:B:538:LYS:O	1:B:540:THR:OG1	2.13	0.64
1:A:252:GLU:OE1	1:A:252:GLU:N	2.30	0.64
1:A:409:VAL:O	1:A:413:LYS:HG3	1.98	0.63
1:A:408:LEU:O	1:A:412:THR:HG23	1.98	0.63
1:B:481:LEU:O	1:B:484:ARG:HG3	1.97	0.63
1:B:198:LEU:HD22	1:B:455:VAL:HG12	1.80	0.62
1:A:48:GLU:O	1:A:52:THR:HG23	2.00	0.62
1:B:409:VAL:O	1:B:413:LYS:HG3	2.00	0.61
1:A:41:LYS:O	1:A:45:GLU:HG3	2.00	0.61
1:A:428:ARG:HD2	1:A:526:GLN:NE2	2.15	0.61
1:A:344:VAL:HG22	1:A:348:ARG:NH1	2.16	0.61
1:B:416:PRO:O	1:B:534:LYS:HE2	2.00	0.60
1:A:37:GLU:CD	1:A:37:GLU:H	2.04	0.60
1:A:302:LEU:HD13	1:A:337:ARG:HH12	1.57	0.60
1:B:110:PRO:HB2	1:B:112:LEU:HG	1.82	0.60
1:A:333:GLU:O	1:A:336:ARG:HG2	2.02	0.60
1:A:464:HIS:HE1	1:A:470:SER:H	1.47	0.60
1:B:240:LYS:O	1:B:244:GLU:HG2	2.02	0.59
1:A:133:THR:O	1:A:137:LYS:HG2	2.01	0.59
1:B:39:HIS:O	1:B:43:VAL:HG23	2.02	0.59
1:B:67:HIS:CG	1:B:99:ASN:HD22	2.20	0.59
1:A:172:ALA:N	1:B:515:THR:O	2.36	0.59
1:A:50:ALA:O	1:A:54:VAL:HG23	2.02	0.58
1:B:61:ASN:HB3	1:B:64:LYS:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLY:C	1:A:87:MET:H	2.07	0.58
1:A:95:GLU:HA	1:A:98:ARG:HG2	1.84	0.58
1:A:240:LYS:O	1:A:244:GLU:HG2	2.03	0.58
1:B:449:ALA:O	1:B:453:LEU:HD12	2.03	0.58
1:A:49:PHE:HZ	1:A:61:ASN:HB3	1.68	0.58
1:A:366:PRO:HB3	1:A:370:TYR:CE2	2.39	0.58
1:A:422:THR:O	1:A:426:VAL:HG23	2.03	0.58
1:A:224:PRO:HB2	1:A:299:PRO:HD3	1.85	0.58
1:A:313:LYS:HZ2	1:A:367:HIS:H	1.51	0.58
1:B:225:LYS:HG2	1:B:299:PRO:HG3	1.84	0.58
1:A:19:PHE:O	1:A:23:VAL:HG23	2.03	0.58
1:A:38:ASP:N	1:A:38:ASP:OD1	2.37	0.58
1:A:265:CYS:SG	1:A:279:CYS:CA	2.91	0.58
1:B:272:SER:HA	1:B:296:ASP:OD2	2.04	0.58
1:A:225:LYS:HG2	1:A:299:PRO:HG3	1.86	0.57
1:B:5:SER:HB2	1:B:62:CYS:HB3	1.86	0.57
1:B:232:SER:HA	1:B:235:VAL:CG1	2.34	0.57
1:B:394:LEU:HD13	1:B:398:LEU:HD12	1.86	0.57
1:B:225:LYS:NZ	1:B:296:ASP:OD2	2.38	0.57
1:A:378:LYS:O	1:A:382:GLU:HG3	2.05	0.57
1:A:504:ALA:O	1:A:508:THR:HG23	2.04	0.57
1:A:302:LEU:HB3	1:A:337:ARG:HH12	1.68	0.57
1:B:222:ARG:HG2	1:B:223:PHE:CE1	2.39	0.57
1:A:31:LEU:HD11	1:A:78:ALA:HB2	1.86	0.56
1:A:366:PRO:HB3	1:A:370:TYR:HE2	1.70	0.56
1:A:224:PRO:HD2	1:A:296:ASP:HB3	1.87	0.56
1:B:386:ASN:O	1:B:390:GLN:HG3	2.05	0.56
1:A:39:HIS:O	1:A:43:VAL:HG23	2.04	0.56
1:B:404:GLN:HG3	1:B:431:GLY:HA3	1.87	0.56
1:A:115:LEU:HG	2:A:800:6AK:C21	2.35	0.56
1:A:121:ASP:O	1:A:125:THR:HG23	2.05	0.56
1:A:264:ILE:C	1:A:266:GLU:H	2.09	0.55
1:B:539:ALA:HB1	1:B:543:GLN:NE2	2.20	0.55
1:B:543:GLN:OE1	1:B:543:GLN:N	2.28	0.55
1:B:132:GLU:OE2	1:B:132:GLU:N	2.39	0.55
1:A:265:CYS:CB	1:A:279:CYS:SG	2.84	0.55
1:A:302:LEU:CG	1:A:337:ARG:HH12	2.14	0.55
1:A:196:GLN:HE22	1:A:242:HIS:HD2	1.55	0.55
1:A:398:LEU:HB3	1:A:402:LYS:HB2	1.88	0.55
1:B:346:LEU:HD12	1:B:346:LEU:H	1.71	0.55
1:A:541:LYS:N	1:A:543:GLN:OE1	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:O	1:A:12:LYS:HG3	2.07	0.55
1:A:302:LEU:HD11	1:A:336:ARG:NH1	2.23	0.55
1:B:9:HIS:CE1	1:B:10:ARG:NH1	2.75	0.54
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.42	0.54
1:B:422:THR:O	1:B:426:VAL:HG23	2.07	0.54
1:B:367:HIS:HA	1:B:370:TYR:CE1	2.42	0.54
1:B:485:ARG:HB3	1:B:486:PRO:HD3	1.89	0.54
1:A:561:ALA:O	1:A:563:ASP:N	2.39	0.54
1:B:88:ALA:O	1:B:91:CYS:HB2	2.08	0.54
1:A:141:GLU:O	1:A:145:ARG:HG3	2.07	0.54
1:A:497:TYR:CD1	1:A:498:VAL:N	2.73	0.54
1:A:325:VAL:HG12	1:A:329:MET:HE3	1.88	0.54
1:B:303:PRO:O	1:B:337:ARG:NH1	2.39	0.54
1:B:342:SER:H	1:B:446:MET:CE	2.21	0.54
1:B:212:LYS:O	1:B:215:ALA:N	2.41	0.54
1:A:540:THR:HA	1:A:544:LEU:HD12	1.90	0.53
1:B:542:GLU:O	1:B:546:ALA:HB2	2.08	0.53
1:B:94:GLN:HA	1:B:98:ARG:HD2	1.91	0.53
1:B:381:VAL:O	1:B:385:GLN:HG3	2.07	0.53
1:B:389:LYS:O	1:B:393:GLU:HG3	2.09	0.53
1:B:61:ASN:CG	1:B:64:LYS:HE2	2.29	0.53
1:A:424:VAL:O	1:A:428:ARG:HG3	2.09	0.53
1:A:34:CYS:HB3	1:A:39:HIS:NE2	2.24	0.53
1:A:500:LYS:O	1:A:500:LYS:HG2	2.08	0.53
1:A:47:THR:O	1:A:51:LYS:HG3	2.09	0.53
1:B:232:SER:HA	1:B:235:VAL:HG12	1.89	0.53
1:B:232:SER:CA	1:B:235:VAL:HG12	2.39	0.53
1:A:171:ALA:HA	1:B:515:THR:HA	1.91	0.52
1:A:420:THR:HG23	1:A:530:VAL:CG2	2.39	0.52
1:A:337:ARG:HG2	1:A:337:ARG:HH11	1.73	0.52
1:B:96:PRO:C	1:B:97:GLU:HG3	2.29	0.52
1:A:231:VAL:O	1:A:235:VAL:HG23	2.09	0.52
1:A:265:CYS:SG	1:A:279:CYS:HA	2.49	0.52
1:A:278:CYS:HB3	1:A:290:ILE:CD1	2.40	0.52
1:A:384:PRO:O	1:A:388:ILE:HG12	2.09	0.52
1:A:430:LEU:O	1:A:433:VAL:HG12	2.09	0.52
1:B:70:PHE:O	1:B:74:LEU:HD12	2.09	0.52
1:B:384:PRO:O	1:B:388:ILE:HG12	2.09	0.52
1:B:516:LEU:HB3	1:B:520:GLU:OE1	2.10	0.52
1:A:375:ASP:OD1	1:A:375:ASP:N	2.42	0.52
1:A:176:ALA:O	1:A:180:PRO:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:PRO:O	1:A:534:LYS:HE2	2.10	0.51
1:B:27:PHE:CE1	1:B:74:LEU:HD11	2.45	0.51
1:B:186:ARG:O	1:B:190:LYS:HG2	2.10	0.51
1:A:278:CYS:HB3	1:A:290:ILE:HD12	1.92	0.51
1:B:100:GLU:HA	1:B:103:LEU:HD12	1.91	0.51
1:B:348:ARG:HH22	1:B:485:ARG:NH2	2.07	0.51
1:A:426:VAL:HG11	1:A:460:LEU:HB2	1.92	0.51
1:B:317:LYS:O	1:B:321:GLU:CB	2.57	0.51
1:B:80:LEU:N	1:B:84:TYR:HH	2.08	0.51
1:B:19:PHE:O	1:B:23:VAL:HG23	2.10	0.51
1:B:481:LEU:HA	1:B:484:ARG:HE	1.76	0.51
1:A:419:SER:OG	1:A:422:THR:HG23	2.11	0.51
1:B:343:VAL:HA	1:B:346:LEU:HD13	1.92	0.51
1:A:117:ARG:HG2	2:A:800:6AK:C13	2.41	0.50
1:A:218:ARG:NH2	1:A:222:ARG:HH11	2.09	0.50
1:A:302:LEU:CB	1:A:337:ARG:HH12	2.25	0.50
1:A:522:GLN:O	1:A:526:GLN:HG2	2.11	0.50
1:B:232:SER:C	1:B:235:VAL:HG12	2.32	0.50
1:B:391:ASN:HD21	1:B:410:ARG:HH22	1.59	0.50
1:A:95:GLU:OE1	1:A:98:ARG:NE	2.34	0.50
1:B:153:GLU:O	1:B:157:PHE:HD1	1.94	0.50
1:B:319:TYR:OH	1:B:358:GLU:OE2	2.26	0.50
1:B:442:GLU:HA	1:B:445:ARG:HB2	1.94	0.50
1:A:394:LEU:O	1:A:398:LEU:HD12	2.12	0.50
1:B:168:CYS:HB2	1:B:178:LEU:HD13	1.94	0.50
1:B:40:VAL:HG12	1:B:44:ASN:OD1	2.12	0.49
1:A:313:LYS:C	1:A:315:VAL:H	2.15	0.49
1:A:366:PRO:CB	1:A:370:TYR:HE2	2.24	0.49
1:A:470:SER:O	1:A:474:THR:HG23	2.11	0.49
1:A:153:GLU:HG2	1:A:257:ARG:HH12	1.77	0.49
1:A:218:ARG:HH21	1:A:222:ARG:HH11	1.59	0.49
1:B:34:CYS:HB3	1:B:39:HIS:HE1	1.76	0.49
1:B:459:GLN:O	1:B:463:LEU:HG	2.12	0.49
1:B:529:LEU:O	1:B:533:VAL:HG23	2.12	0.49
1:A:175:ALA:O	1:A:179:LEU:HD12	2.13	0.49
1:A:151:ALA:O	1:A:154:LEU:N	2.46	0.49
1:A:276:LYS:HE3	1:A:280:GLU:OE2	2.12	0.49
1:B:265:CYS:SG	1:B:286:LYS:HE2	2.52	0.49
1:B:378:LYS:N	1:B:379:PRO:HD2	2.28	0.49
1:A:196:GLN:HE22	1:A:242:HIS:CD2	2.30	0.49
1:A:164:ALA:O	1:A:168:CYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LYS:HA	1:B:381:VAL:HG22	1.94	0.48
1:B:118:PRO:HG2	1:B:123:MET:CG	2.43	0.48
1:A:153:GLU:O	1:A:156:PHE:HB3	2.13	0.48
1:A:464:HIS:CE1	1:A:469:VAL:H	2.30	0.48
1:B:42:LEU:HD23	1:B:73:LYS:HE3	1.94	0.48
1:A:49:PHE:CZ	1:A:61:ASN:HB3	2.48	0.48
1:B:27:PHE:HB3	1:B:39:HIS:HD2	1.79	0.48
1:A:408:LEU:HD23	1:A:408:LEU:HA	1.40	0.48
1:A:531:GLU:OE1	1:A:535:HIS:HE1	1.96	0.48
1:A:298:MET:SD	1:A:337:ARG:HA	2.53	0.48
1:B:37:GLU:CD	1:B:37:GLU:H	2.17	0.48
1:B:404:GLN:HG2	1:B:428:ARG:HA	1.96	0.48
1:B:550:ASP:O	1:B:554:PHE:CB	2.61	0.48
1:B:400:GLU:OE1	1:B:435:SER:OG	2.20	0.48
1:B:449:ALA:O	1:B:452:TYR:N	2.46	0.48
1:A:106:LYS:HD3	1:A:147:PRO:HB2	1.96	0.48
1:B:79:THR:N	1:B:84:TYR:OH	2.47	0.48
1:B:440:HIS:ND1	1:B:441:PRO:HD2	2.29	0.48
1:A:224:PRO:CD	1:A:296:ASP:HB3	2.44	0.48
1:B:330:PHE:HE2	1:B:350:ALA:HA	1.77	0.48
1:B:332:TYR:HD1	1:B:333:GLU:HG2	1.78	0.47
1:B:541:LYS:H	1:B:544:LEU:HG	1.79	0.47
1:B:543:GLN:O	1:B:546:ALA:HB3	2.14	0.47
1:B:420:THR:HG23	1:B:530:VAL:CG2	2.44	0.47
1:B:149:PHE:CD1	1:B:154:LEU:HB2	2.49	0.47
1:B:408:LEU:HD21	1:B:427:SER:HB2	1.94	0.47
1:B:452:TYR:O	1:B:455:VAL:HG22	2.14	0.47
1:A:485:ARG:HB3	1:A:486:PRO:HD3	1.95	0.47
1:B:217:ALA:HB2	1:B:331:LEU:HD21	1.96	0.47
1:A:18:ASN:HA	1:A:21:ALA:HB3	1.96	0.47
1:A:529:LEU:O	1:A:533:VAL:HG23	2.14	0.47
1:B:10:ARG:HH21	1:B:252:GLU:CB	2.28	0.47
1:B:196:GLN:O	1:B:196:GLN:HG3	2.14	0.47
1:B:500:LYS:H	1:B:535:HIS:HA	1.78	0.47
1:A:413:LYS:HZ1	1:A:537:PRO:HA	1.79	0.47
1:B:230:GLU:O	1:B:234:LEU:HG	2.15	0.47
1:B:458:ASN:O	1:B:462:VAL:HG13	2.15	0.47
1:A:306:ALA:O	1:A:311:GLU:HG3	2.15	0.46
1:A:561:ALA:C	1:A:563:ASP:N	2.66	0.46
1:B:84:TYR:CD1	1:B:85:GLY:N	2.83	0.46
1:B:77:VAL:HG22	1:B:77:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:HG2	1:A:223:PHE:CD1	2.50	0.46
1:B:140:TYR:O	1:B:144:ARG:HG2	2.15	0.46
1:A:218:ARG:O	1:A:218:ARG:NH1	2.49	0.46
1:A:540:THR:HB	1:A:544:LEU:CD1	2.27	0.46
1:A:340:ASP:OD1	1:A:340:ASP:N	2.31	0.46
1:B:352:THR:O	1:B:356:THR:HG23	2.15	0.46
1:A:341:TYR:HA	1:A:446:MET:CE	2.46	0.46
1:A:418:VAL:HG23	1:A:423:LEU:HG	1.98	0.46
1:B:10:ARG:HE	1:B:252:GLU:HB3	1.81	0.46
1:A:36:PHE:CE2	1:A:137:LYS:HD3	2.51	0.46
1:A:215:ALA:CB	1:A:235:VAL:HG13	2.44	0.46
1:A:538:LYS:O	1:A:540:THR:HG23	2.16	0.46
1:B:10:ARG:HH21	1:B:252:GLU:HB3	1.80	0.46
1:B:342:SER:H	1:B:446:MET:HE3	1.80	0.46
1:A:418:VAL:O	1:A:534:LYS:NZ	2.35	0.45
1:A:179:LEU:HD23	2:A:800:6AK:C37	2.46	0.45
1:A:237:ASP:O	1:A:240:LYS:HB3	2.15	0.45
1:B:38:ASP:O	1:B:41:LYS:HB3	2.16	0.45
1:B:268:GLN:HE22	1:B:276:LYS:HA	1.81	0.45
1:B:447:PRO:O	1:B:451:ASP:HB2	2.17	0.45
1:A:32:GLN:NE2	1:A:110:PRO:HG3	2.32	0.45
1:B:196:GLN:HA	1:B:199:LYS:HG3	1.99	0.45
1:B:223:PHE:CD1	1:B:272:SER:HB2	2.52	0.45
1:B:340:ASP:OD1	1:B:340:ASP:N	2.42	0.45
1:B:281:LYS:HB3	1:B:285:GLU:HB3	1.99	0.45
1:B:513:ILE:HA	1:B:516:LEU:HD12	1.99	0.45
1:B:146:HIS:CD2	2:B:802:6AK:CL2	3.07	0.45
1:B:375:ASP:C	1:B:377:PHE:N	2.70	0.45
1:A:49:PHE:HD1	1:A:49:PHE:O	2.00	0.45
1:B:5:SER:CB	1:B:62:CYS:HB3	2.45	0.45
1:B:42:LEU:HD22	1:B:73:LYS:HG3	1.99	0.45
1:B:98:ARG:O	1:B:101:CYS:HB3	2.17	0.45
1:A:541:LYS:H	1:A:543:GLN:CD	2.18	0.44
1:B:73:LYS:NZ	1:B:76:THR:HG21	2.32	0.44
1:A:323:LYS:C	1:A:327:LEU:HD12	2.38	0.44
1:B:410:ARG:HD2	1:B:411:TYR:CE1	2.53	0.44
1:A:472:ARG:NH2	1:A:492:GLU:O	2.51	0.44
1:B:550:ASP:O	1:B:554:PHE:HB3	2.17	0.44
1:A:119:GLU:OE1	1:A:119:GLU:N	2.51	0.44
1:A:94:GLN:C	1:A:98:ARG:HG2	2.38	0.44
1:A:98:ARG:HG3	1:A:99:ASN:H	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:ALA:HB1	1:B:235:VAL:HG23	1.99	0.44
1:B:123:MET:HG2	2:B:802:6AK:C16	2.47	0.44
1:B:420:THR:HG21	1:B:527:THR:HG23	2.00	0.44
1:A:27:PHE:CD1	1:A:74:LEU:HD21	2.53	0.44
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.80	0.44
1:B:78:ALA:C	1:B:84:TYR:OH	2.57	0.44
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.70	0.43
1:A:417:GLN:H	1:A:417:GLN:CD	2.19	0.43
1:B:375:ASP:C	1:B:377:PHE:H	2.22	0.43
1:A:99:ASN:O	1:A:103:LEU:HD12	2.18	0.43
1:A:428:ARG:HD2	1:A:526:GLN:HE22	1.81	0.43
1:B:86:GLU:OE1	1:B:105:HIS:NE2	2.52	0.43
1:B:348:ARG:NH1	1:B:450:GLU:OE2	2.50	0.43
1:A:217:ALA:HB3	1:A:343:VAL:HG13	2.01	0.43
1:A:367:HIS:O	1:A:371:ALA:HB2	2.18	0.43
1:A:217:ALA:O	1:A:221:GLN:HG3	2.19	0.43
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.84	0.43
1:A:342:SER:H	1:A:446:MET:CE	2.32	0.43
1:A:363:ALA:HB3	1:A:369:CYS:SG	2.58	0.43
1:A:384:PRO:O	1:A:387:LEU:N	2.51	0.43
1:B:410:ARG:HD2	1:B:411:TYR:HE1	1.83	0.43
1:B:453:LEU:HD12	1:B:453:LEU:H	1.84	0.43
1:A:95:GLU:CA	1:A:98:ARG:HG2	2.47	0.43
1:A:218:ARG:HH22	1:A:295:ASN:HD21	1.65	0.43
1:A:401:TYR:O	1:A:404:GLN:HB2	2.19	0.43
1:B:152:PRO:HB2	1:B:257:ARG:NH1	2.29	0.43
1:A:554:PHE:HE1	1:A:558:CYS:SG	2.42	0.43
1:A:134:PHE:O	1:A:137:LYS:HB2	2.19	0.43
1:A:222:ARG:O	1:A:224:PRO:HD3	2.19	0.43
1:A:367:HIS:HA	1:A:370:TYR:CD1	2.53	0.43
1:A:153:GLU:HG2	1:A:257:ARG:NH1	2.33	0.42
1:B:67:HIS:CD2	1:B:99:ASN:ND2	2.76	0.42
1:B:221:GLN:HG2	1:B:335:ALA:O	2.19	0.42
1:A:554:PHE:HZ	1:A:568:PHE:HA	1.84	0.42
1:A:554:PHE:CZ	1:A:568:PHE:HA	2.54	0.42
1:B:332:TYR:OH	1:B:336:ARG:NH2	2.52	0.42
1:B:530:VAL:O	1:B:534:LYS:HG3	2.19	0.42
1:A:264:ILE:C	1:A:266:GLU:N	2.71	0.42
1:A:366:PRO:HB2	1:A:370:TYR:CE2	2.53	0.42
1:B:511:ALA:HB2	1:B:565:GLU:HB2	1.99	0.42
1:A:372:LYS:HG2	1:A:375:ASP:OD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:CYS:O	1:B:366:PRO:HA	2.18	0.42
1:B:540:THR:HG23	1:B:544:LEU:HD11	2.00	0.42
1:B:544:LEU:C	1:B:546:ALA:N	2.73	0.42
1:B:251:LEU:H	1:B:251:LEU:HD12	1.84	0.42
1:A:373:VAL:HG13	1:A:374:PHE:CD1	2.54	0.42
1:B:27:PHE:HB3	1:B:39:HIS:CD2	2.53	0.42
1:B:564:LYS:C	1:B:566:THR:N	2.73	0.42
1:A:302:LEU:HD22	1:A:302:LEU:HA	1.82	0.42
1:A:337:ARG:HH11	1:A:337:ARG:CG	2.33	0.42
1:A:384:PRO:O	1:A:385:GLN:C	2.56	0.42
1:A:412:THR:CG2	1:A:423:LEU:HD13	2.40	0.42
1:B:135:LEU:HD11	1:B:158:ALA:HB1	2.02	0.42
1:B:276:LYS:H	1:B:276:LYS:HG2	1.64	0.42
1:B:325:VAL:O	1:B:329:MET:HB2	2.20	0.42
1:A:286:LYS:O	1:A:290:ILE:HD13	2.20	0.42
1:A:288:HIS:O	1:A:292:GLU:HG3	2.20	0.42
1:B:231:VAL:O	1:B:235:VAL:CG1	2.66	0.42
1:B:344:VAL:HG12	1:B:451:ASP:OD1	2.20	0.42
1:B:227:GLU:HG2	1:B:228:PHE:N	2.34	0.41
1:B:394:LEU:HD13	1:B:398:LEU:CD1	2.50	0.41
1:B:540:THR:HA	1:B:544:LEU:HG	2.01	0.41
1:A:325:VAL:O	1:A:329:MET:HB2	2.20	0.41
1:A:85:GLY:C	1:A:87:MET:N	2.73	0.41
1:B:348:ARG:HH22	1:B:485:ARG:HH21	1.69	0.41
1:A:189:GLY:HA3	2:A:800:6AK:C24	2.50	0.41
1:A:313:LYS:CG	1:A:367:HIS:HB2	2.50	0.41
1:A:405:ASN:O	1:A:409:VAL:HG23	2.20	0.41
1:B:281:LYS:HB3	1:B:285:GLU:CB	2.51	0.41
1:B:426:VAL:HG11	1:B:460:LEU:HB2	2.03	0.41
1:A:554:PHE:CE1	1:A:558:CYS:SG	3.13	0.41
1:B:157:PHE:CE2	1:B:189:GLY:HA2	2.55	0.41
1:B:405:ASN:O	1:B:408:LEU:HB2	2.20	0.41
1:B:44:ASN:O	1:B:48:GLU:HG2	2.20	0.41
1:B:225:LYS:NZ	1:B:296:ASP:CG	2.73	0.41
1:B:309:PHE:CE1	1:B:326:PHE:HE1	2.39	0.41
1:B:329:MET:O	1:B:332:TYR:HB3	2.19	0.41
1:B:507:PHE:HZ	1:B:532:LEU:HA	1.85	0.41
1:A:464:HIS:HE1	1:A:469:VAL:H	1.69	0.41
1:A:108:ASP:OD1	1:A:197:ARG:NE	2.53	0.41
1:A:306:ALA:C	1:A:311:GLU:HG3	2.41	0.41
1:A:351:LYS:O	1:A:355:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ALA:HB3	1:B:62:CYS:SG	2.61	0.41
1:A:55:ALA:O	1:A:56:ASP:HB3	2.21	0.41
1:A:179:LEU:HD12	1:A:179:LEU:H	1.86	0.41
1:A:376:GLU:H	1:A:376:GLU:HG2	1.62	0.41
1:B:87:MET:HE2	1:B:105:HIS:HB3	2.02	0.41
1:B:184:GLU:O	1:B:188:GLU:HB2	2.21	0.41
1:B:541:LYS:N	1:B:544:LEU:HG	2.36	0.41
1:B:9:HIS:CE1	1:B:10:ARG:HH11	2.38	0.41
1:B:51:LYS:CA	1:B:54:VAL:HG12	2.39	0.41
1:B:186:ARG:HA	2:B:802:6AK:C27	2.51	0.41
1:B:386:ASN:HD21	1:B:390:GLN:HE21	1.69	0.41
1:A:381:VAL:O	1:A:385:GLN:HG3	2.20	0.40
1:B:327:LEU:O	1:B:330:PHE:N	2.53	0.40
1:A:94:GLN:O	1:A:98:ARG:HB3	2.20	0.40
1:A:439:LYS:HG2	1:A:440:HIS:CD2	2.57	0.40
1:A:196:GLN:NE2	1:A:242:HIS:HD2	2.17	0.40
1:A:519:LYS:O	1:A:523:ILE:HG13	2.22	0.40
1:B:217:ALA:O	1:B:221:GLN:HG3	2.21	0.40
1:B:561:ALA:C	1:B:563:ASP:H	2.24	0.40
1:B:276:LYS:O	1:B:280:GLU:HG2	2.21	0.40
1:B:351:LYS:O	1:B:355:THR:HG23	2.21	0.40
1:A:85:GLY:O	1:A:87:MET:N	2.54	0.40
1:B:99:ASN:O	1:B:103:LEU:HG	2.22	0.40
1:B:272:SER:HB3	1:B:275:LEU:HG	2.03	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	566/609 (93%)	506 (89%)	50 (9%)	10 (2%)	8 21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	563/609 (92%)	505 (90%)	50 (9%)	8 (1%)	11 28
All	All	1129/1218 (93%)	1011 (90%)	100 (9%)	18 (2%)	9 24

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	78	ALA
1	B	60	GLU
1	B	439	LYS
1	A	57	GLU
1	A	171	ALA
1	A	86	GLU
1	A	563	ASP
1	B	96	PRO
1	B	212	LYS
1	B	541	LYS
1	A	5	SER
1	A	265	CYS
1	B	113	PRO
1	A	479	GLU
1	A	538	LYS
1	B	59	ALA
1	B	95	GLU

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	446/533 (84%)	424 (95%)	22 (5%)	25 52
1	B	448/533 (84%)	434 (97%)	14 (3%)	40 69
All	All	894/1066 (84%)	858 (96%)	36 (4%)	31 60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	31	LEU
1	A	33	GLN
1	A	37	GLU
1	A	38	ASP
1	A	49	PHE
1	A	58	SER
1	A	61	ASN
1	A	98	ARG
1	A	209	ARG
1	A	265	CYS
1	A	270	SER
1	A	274	LYS
1	A	302	LEU
1	A	334	TYR
1	A	375	ASP
1	A	422	THR
1	A	471	ASP
1	A	481	LEU
1	A	482	VAL
1	A	520	GLU
1	A	526	GLN
1	B	18	ASN
1	B	34	CYS
1	B	38	ASP
1	B	51	LYS
1	B	89	ASP
1	B	232	SER
1	B	302	LEU
1	B	334	TYR
1	B	370	TYR
1	B	378	LYS
1	B	440	HIS
1	B	444	LYS
1	B	471	ASP
1	B	518	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	146	HIS
1	A	242	HIS

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Mol	Chain	Res	Type
1	A	295	ASN
1	A	429	ASN
1	A	464	HIS
1	A	526	GLN
1	B	9	HIS
1	B	32	GLN
1	B	39	HIS
1	B	99	ASN
1	B	104	GLN
1	B	204	GLN
1	B	268	GLN
1	B	386	ASN
1	B	390	GLN
1	B	391	ASN

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)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	B	801	-	4,4,4	1.07	0	6,6,6	1.55	1 (16%)
3	PO4	A	801	-	4,4,4	1.12	0	6,6,6	2.59	3 (50%)
2	6AK	A	800	-	47,56,56	1.76	8 (17%)	56,85,85	2.82	22 (39%)
2	6AK	B	802	-	47,56,56	1.45	6 (12%)	56,85,85	2.75	11 (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	6AK	A	800	-	-	7/19/33/33	0/6/7/7
2	6AK	B	802	-	-	5/19/33/33	0/6/7/7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	6AK	C14-N02	-5.76	1.45	1.49
2	A	800	6AK	C12-N01	5.33	1.43	1.37
2	B	802	6AK	C12-N01	5.24	1.43	1.37
2	A	800	6AK	C08-C07	-3.37	1.46	1.52
2	B	802	6AK	C30-C31	3.33	1.43	1.37
2	A	800	6AK	C19-C02	-3.19	1.48	1.50
2	B	802	6AK	C19-C02	-3.12	1.48	1.50
2	B	802	6AK	C05-C04	3.04	1.43	1.36
2	A	800	6AK	C13-N01	2.74	1.51	1.47
2	A	800	6AK	C30-C31	2.66	1.42	1.37
2	A	800	6AK	O03-C32	2.37	1.29	1.22
2	B	802	6AK	O03-C32	2.29	1.29	1.22
2	B	802	6AK	C31-C32	2.23	1.54	1.49
2	A	800	6AK	C21-C20	-2.03	1.46	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	6AK	C15-C14-N02	-11.37	102.27	111.18
2	B	802	6AK	C14-C15-C13	-11.04	100.64	112.31
2	B	802	6AK	O02-C12-N01	8.34	129.52	121.01
2	B	802	6AK	C11-C12-N01	-7.69	107.48	119.53
2	A	800	6AK	C09-C08-C07	-7.21	98.71	113.24
2	A	800	6AK	C11-C12-N01	-6.30	109.66	119.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	6AK	C19-C02-C03	-5.25	115.34	121.63
3	A	801	PO4	O4-P-O2	-5.00	91.91	107.97
2	A	800	6AK	O02-C12-N01	4.50	125.60	121.01
2	A	800	6AK	C14-C15-C13	-4.33	107.74	112.31
2	B	802	6AK	C16-N03-C17	-4.18	123.35	128.82
2	B	802	6AK	C15-C14-N02	4.05	114.36	111.18
2	B	802	6AK	C09-C08-C07	-3.99	105.19	113.24
2	B	802	6AK	C30-C31-C32	3.98	129.14	120.67
2	A	800	6AK	C02-C19-C20	3.95	134.86	127.52
2	A	800	6AK	C33-C31-C32	-3.81	113.08	119.98
2	B	802	6AK	C33-C31-C32	-3.72	113.24	119.98
2	B	802	6AK	O01-C10-C09	-3.45	95.50	108.33
2	A	800	6AK	C23-C22-CL2	3.23	124.58	118.19
2	A	800	6AK	O01-C10-C09	-3.22	96.36	108.33
2	A	800	6AK	C29-C28-C27	3.17	125.35	119.49
2	A	800	6AK	C28-C22-CL2	-3.05	112.17	118.19
3	A	801	PO4	O4-P-O3	2.96	117.48	107.97
2	A	800	6AK	C02-C19-C17	-2.96	122.02	127.52
2	A	800	6AK	C04-C05-C06	-2.75	117.30	121.13
2	A	800	6AK	C10-O01-C26	2.73	125.05	117.93
2	A	800	6AK	C16-N03-C17	-2.54	125.50	128.82
3	B	801	PO4	O4-P-O2	2.49	115.95	107.97
2	A	800	6AK	C26-C27-C28	2.47	123.25	120.59
2	A	800	6AK	C30-C31-C32	2.47	125.92	120.67
2	A	800	6AK	C19-C02-C03	-2.34	118.83	121.63
2	A	800	6AK	C04-C03-CL	-2.31	113.77	118.41
2	A	800	6AK	C05-C06-C01	2.26	120.95	116.73
3	A	801	PO4	O2-P-O1	2.25	119.11	110.89
2	A	800	6AK	O01-C26-C27	2.21	130.46	119.86
2	A	800	6AK	C13-N01-C34	2.09	119.57	115.62
2	B	802	6AK	C10-O01-C26	2.03	123.23	117.93

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	802	6AK	C07-C08-C09-C10
2	B	802	6AK	C08-C09-C10-O01
2	A	800	6AK	C33-C31-C32-O04
2	A	800	6AK	C08-C09-C10-O01
2	A	800	6AK	C30-C31-C32-O04
2	A	800	6AK	C33-C31-C32-O03

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Mol	Chain	Res	Type	Atoms
2	A	800	6AK	C30-C31-C32-O03
2	B	802	6AK	C33-C31-C32-O04
2	A	800	6AK	C35-C34-N01-C12
2	B	802	6AK	C30-C31-C32-O04
2	A	800	6AK	C07-C08-C09-C10
2	B	802	6AK	C33-C31-C32-O03

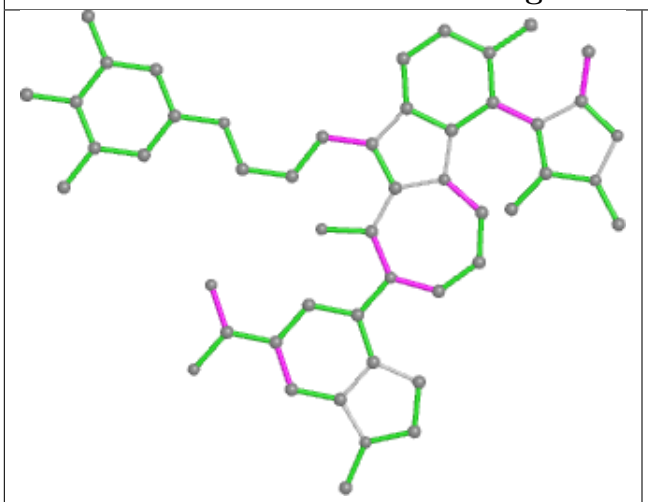
There are no ring outliers.

3 monomers are involved in 9 short contacts:

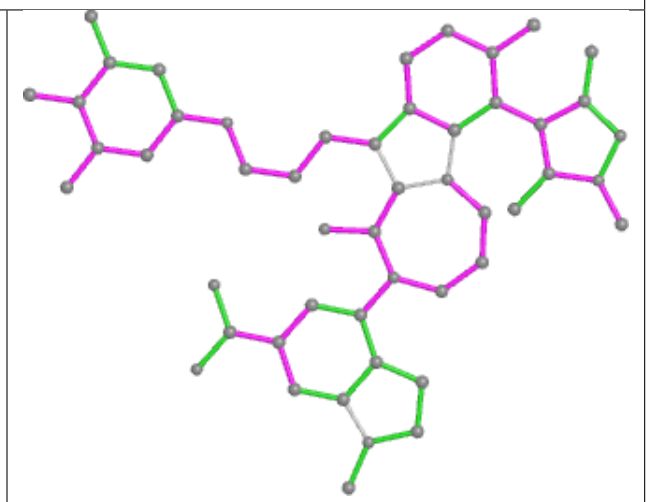
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	PO4	1	0
2	A	800	6AK	4	0
2	B	802	6AK	4	0

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

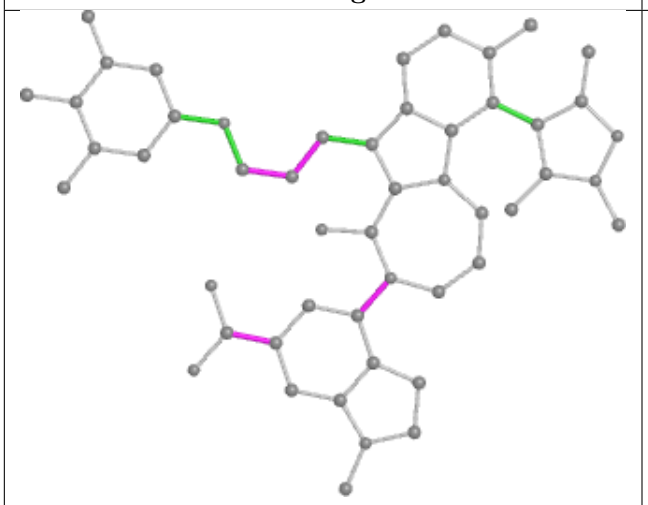
Ligand 6AK A 800



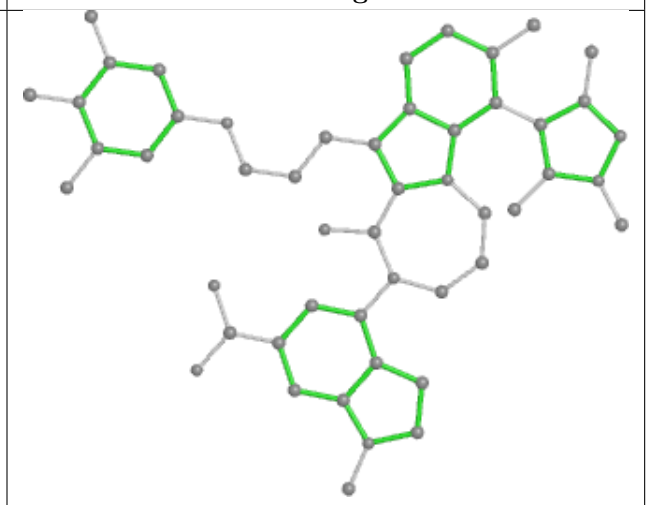
Bond lengths



Bond angles

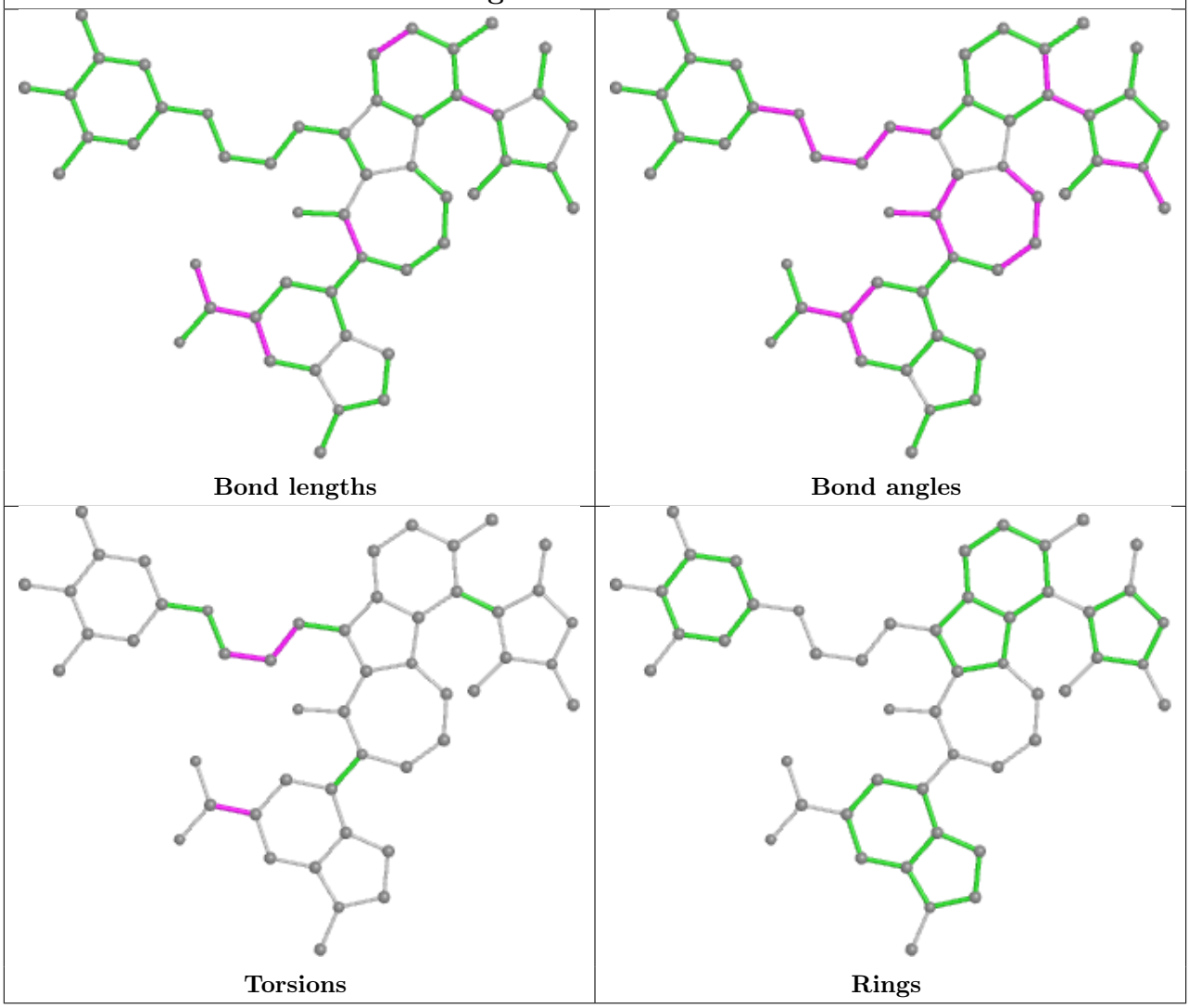


Torsions



Rings

Ligand 6AK B 802



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	568/609 (93%)	0.03	13 (2%)	60	62	36, 64, 110, 134	0
1	B	565/609 (92%)	0.06	14 (2%)	57	59	42, 70, 110, 139	0
All	All	1133/1218 (93%)	0.04	27 (2%)	59	60	36, 67, 110, 139	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ALA	8.0
1	A	79	THR	5.6
1	B	353	TYR	4.2
1	B	363	ALA	4.2
1	B	507	PHE	4.2
1	A	84	TYR	4.1
1	A	87	MET	4.0
1	B	31	LEU	3.9
1	A	539	ALA	3.6
1	A	509	PHE	3.4
1	A	551	PHE	3.4
1	B	96	PRO	3.2
1	A	507	PHE	3.1
1	B	374	PHE	3.0
1	A	314	ASP	2.9
1	B	380	LEU	2.6
1	B	330	PHE	2.6
1	B	537	PRO	2.5
1	B	70	PHE	2.5
1	B	294	GLU	2.4
1	A	540	THR	2.4
1	B	79	THR	2.3
1	B	278	CYS	2.3
1	A	8	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	319	TYR	2.2
1	A	96	PRO	2.2
1	B	78	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

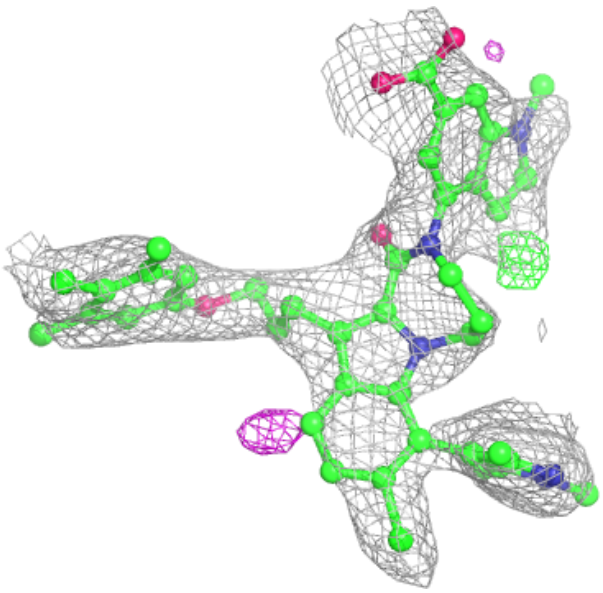
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

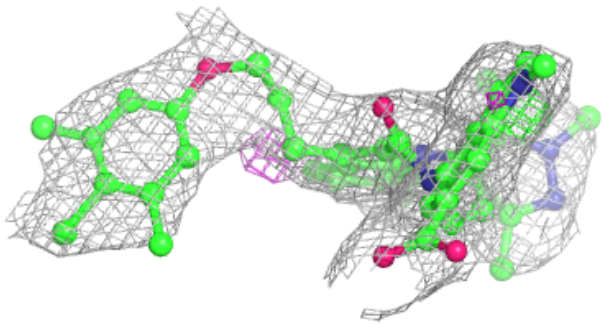
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6AK	A	800	50/50	0.86	0.30	26,61,87,91	50
3	PO4	A	801	5/5	0.89	0.16	37,47,60,77	0
2	6AK	B	802	50/50	0.90	0.32	23,51,61,88	50
3	PO4	B	801	5/5	0.96	0.11	30,42,55,56	0

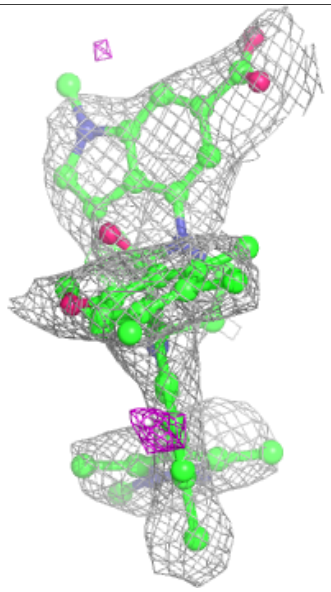
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6AK A 800:

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

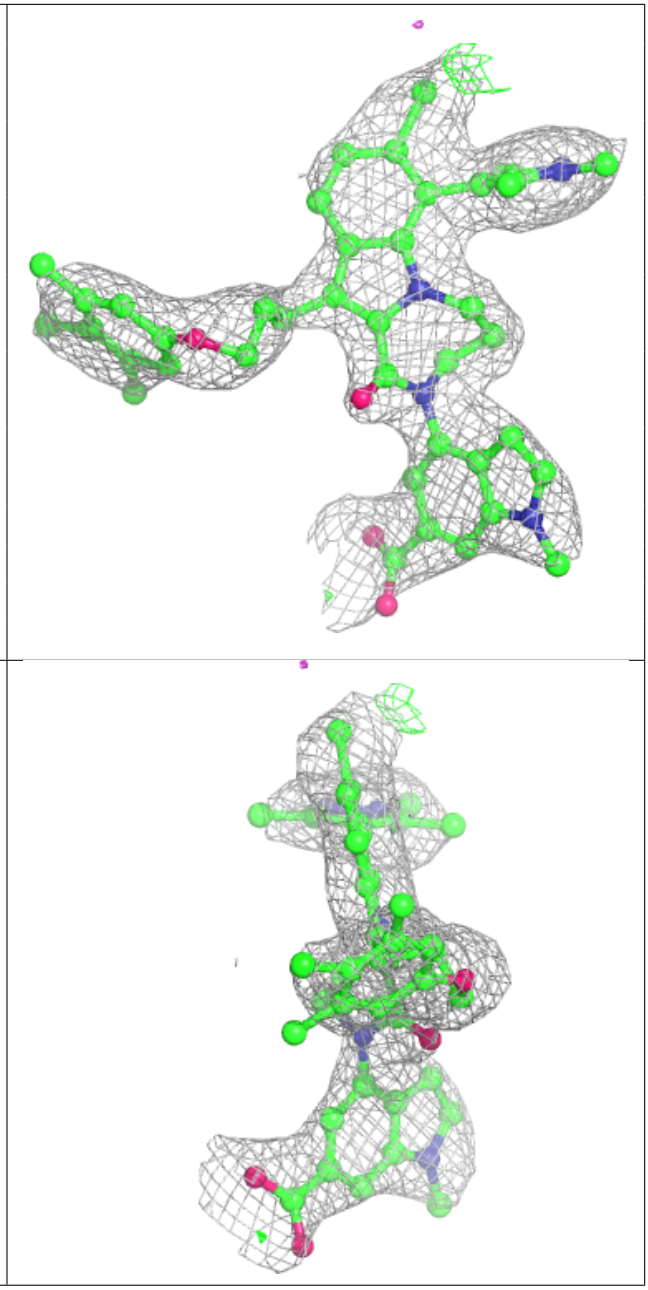






Electron density around 6AK B 802:

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



6.5 Other polymers (i)

There are no such residues in this entry.