Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:44 PM UTC

PDB ID	:	1NHV / pdb_00001nhv
Title	:	Hepatitis C virus RNA polymerase in complex with non-nucleoside analogue inhibitor
Authors	:	Wang, M.; Ng, K.K.S.; Cherney, M.M.; Chan, L.; Yannopoulos, C.G.; Bedard, J.; Morin, N.; Nguyen-Ba, N.; Alaoui-Ismaili, M.H.; Bethell, R.C.; James, M.N.G.
Deposited on	:	2002-12-19
Resolution	:	2.90 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 ⓘ 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 (1)) were used in the production of this report:

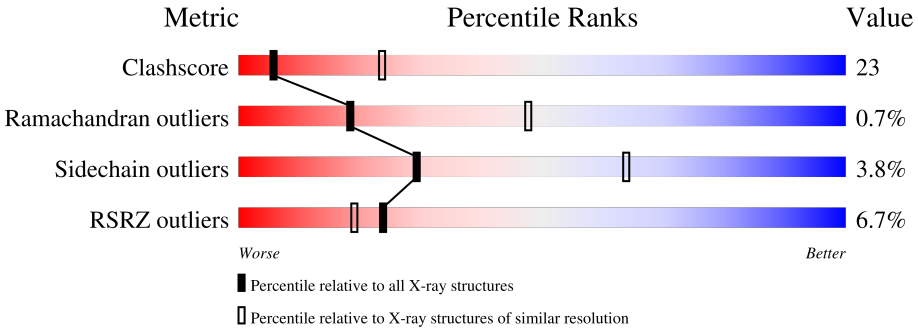
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	578	6% 52% 42%
1	B	578	7% 56% 38%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8779 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.

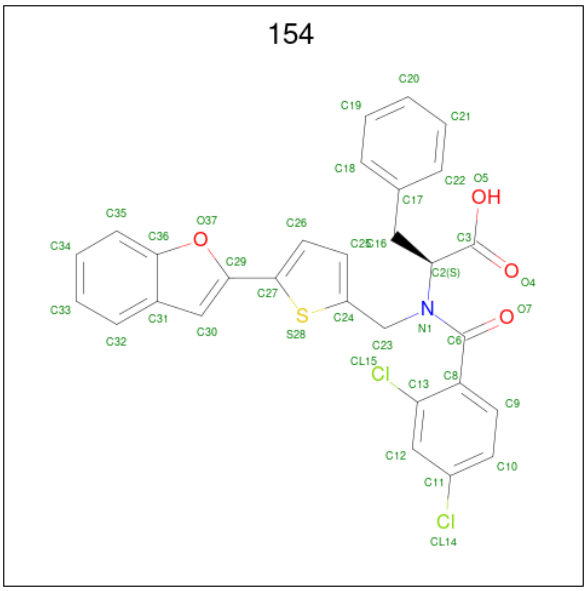
- Molecule 1 is a protein called HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	558	Total	C	N	O	S	0	0	0
			4340	2738	765	806	31			
1	B	561	Total	C	N	O	S	0	0	0
			4365	2753	771	810	31			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ALA	-	expression tag	UNP P26663
A	-6	SER	-	expression tag	UNP P26663
A	-5	HIS	-	expression tag	UNP P26663
A	-4	HIS	-	expression tag	UNP P26663
A	-3	HIS	-	expression tag	UNP P26663
A	-2	HIS	-	expression tag	UNP P26663
A	-1	HIS	-	expression tag	UNP P26663
A	0	HIS	-	expression tag	UNP P26663
B	-7	ALA	-	expression tag	UNP P26663
B	-6	SER	-	expression tag	UNP P26663
B	-5	HIS	-	expression tag	UNP P26663
B	-4	HIS	-	expression tag	UNP P26663
B	-3	HIS	-	expression tag	UNP P26663
B	-2	HIS	-	expression tag	UNP P26663
B	-1	HIS	-	expression tag	UNP P26663
B	0	HIS	-	expression tag	UNP P26663

- Molecule 2 is (2S)-2-[(5-BENZOFURAN-2-YL-THIOPHEN-2-YLMETHYL)-(2,4-DICHLORO-BENZOYL)-AMINO]-3-PHENYL-PROPIONIC ACID (CCD ID: 154) (formula: $C_{29}H_{21}Cl_2NO_4S$).



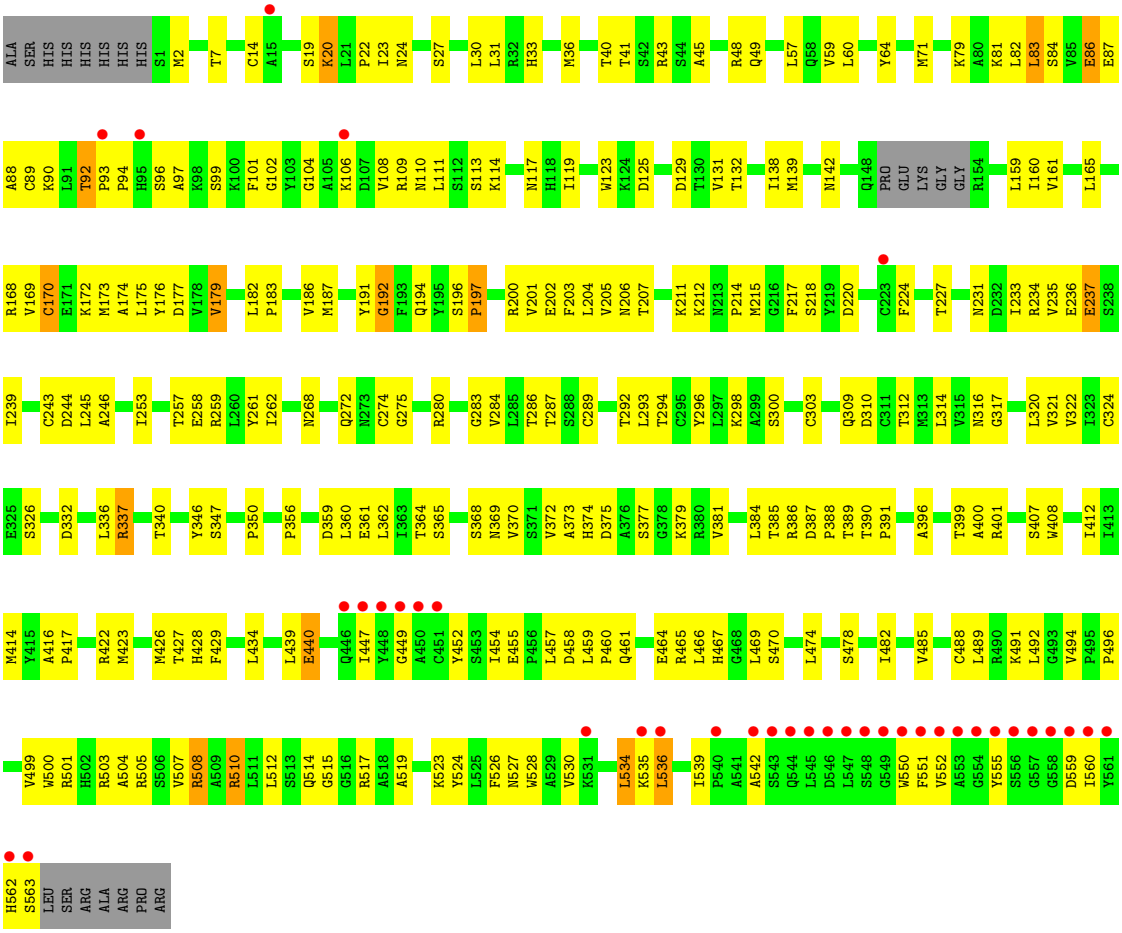
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			37	29	2	1	4	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			37	29	2	1	4	1		

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.

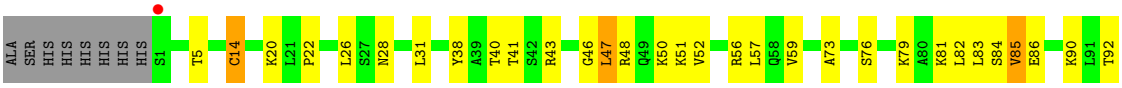
• Molecule 1: HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE

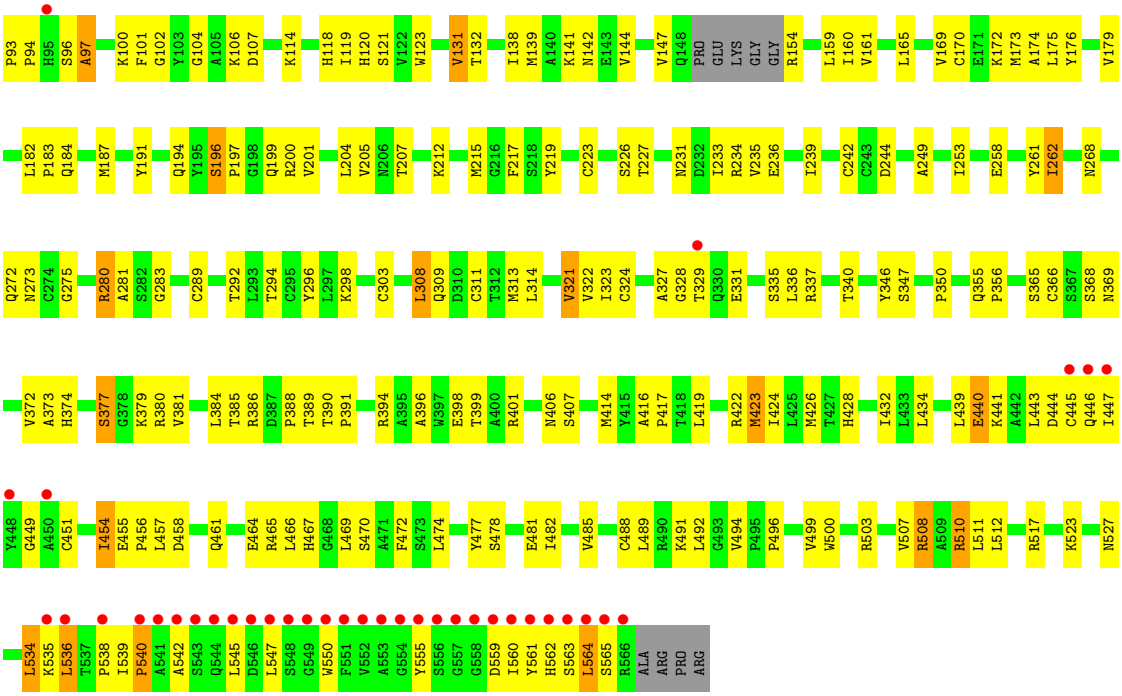
Chain A:



• Molecule 1: HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE

Chain B:




P93 P94 H95 S96 A97 K100 F101 G102 Y103 G104 A105 K106 D107 K114 H118 I119 H120 S121 V122 W123 V131 T132 I138 M139 A140 K141 N142 E143 V144 V147 Q148 PRO GLU LYS GLY GLY R154 L159 I160 V161 L165 V169 C170 E171 K172 M173 A174 L175 Y176 V179
L182 P183 Q184 M187 Y191 Q194 Y195 S196 P197 G198 Q199 R200 V201 L204 V205 N206 T207 K212 M215 G216 F217 S218 Y219 C223 S226 T227 N231 D232 I233 R234 V235 E236 I239 C242 C243 D244 A249 I253 E258 Y261 I262 N268
Q272 N273 C274 G275 R280 A281 S282 G283 C289 T292 L293 T294 C295 Y296 L297 K298 C303 L308 Q309 D310 C311 T312 M313 L314 V321 V322 I323 C324 A327 G328 T329 Q330 E331 S335 L336 R337 T340 Y346 S347 P350 Q355 P356 S365 C366 S367 S368 N369
V372 A373 H374 S377 G378 K379 R380 V381 L384 T385 R386 D387 P388 T389 T390 P391 R394 A395 A396 W397 E398 T399 A400 R401 N406 S407 M414 Y415 A416 P417 T418 L419 R422 M423 I424 L425 M426 T427 H428 I432 L433 L434 L439 E440 K441 A442 L443 D444 C445 Q446 I447
Y448 G449 A450 C451 I454 E455 P456 L457 D458 Q461 E464 R465 L466 H467 G468 L469 S470 A471 F472 S473 L474 Y477 S478 E481 I482 V485 C488 L489 R490 K491 L492 G493 V494 P495 P496 V499 W500 R503 V507 R508 A509 R510 L511 L512 R517 K523 N527
L534 K535 L536 T537 P538 I539 P540 A541 A542 S543 Q544 L545 D546 L547 S548 G549 W550 F551 V552 A553 G554 Y555 S556 G557 G558 D559 I560 Y561 H562 S563 L564 S565 R566 ALA ARG PRO ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	85.50Å 107.83Å 126.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.74 – 2.90 39.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (39.74-2.90) 94.2 (39.74-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.90Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.280 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 53.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8779	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.98 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5035e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 154

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	0.49	1/4434 (0.0%)	1.01	17/6017 (0.3%)
1	B	0.50	0/4459	0.98	13/6050 (0.2%)
All	All	0.50	1/8893 (0.0%)	0.99	30/12067 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	MET	SD-CE	5.24	1.92	1.79

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	552	VAL	N-CA-C	-6.96	106.71	113.53
1	A	212	LYS	N-CA-C	-6.74	103.86	111.07
1	A	244	ASP	N-CA-C	-6.68	98.31	108.67
1	B	212	LYS	N-CA-C	-6.68	103.69	110.97
1	B	100	LYS	N-CA-C	-6.62	105.19	113.20
1	A	196	SER	N-CA-C	-6.59	100.50	110.39
1	A	224	PHE	N-CA-C	6.38	119.05	111.33
1	A	218	SER	N-CA-C	-5.87	101.05	110.14
1	B	423	MET	N-CA-C	5.77	118.52	111.82
1	B	280	ARG	N-CA-C	5.74	118.66	110.10
1	B	508	ARG	N-CA-C	-5.71	104.97	111.14
1	B	28	ASN	N-CA-C	5.69	119.74	112.34
1	B	281	ALA	N-CA-C	-5.64	101.28	110.20
1	B	196	SER	N-CA-C	-5.60	102.86	110.36
1	A	192	GLY	N-CA-C	5.59	120.92	114.16
1	B	454	ILE	N-CA-C	5.48	116.37	108.48
1	B	424	ILE	N-CA-C	5.43	116.58	111.48
1	A	92	THR	CA-C-N	5.41	125.95	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	92	THR	C-N-CA	5.41	125.95	120.38
1	A	454	ILE	N-CA-C	5.39	116.43	108.45
1	A	246	ALA	CA-C-N	5.37	125.44	119.32
1	A	246	ALA	C-N-CA	5.37	125.44	119.32
1	A	300	SER	N-CA-C	-5.37	105.09	111.69
1	A	508	ARG	N-CA-C	-5.35	105.34	111.07
1	B	51	LYS	N-CA-C	5.26	118.80	112.38
1	A	84	SER	N-CA-C	-5.16	102.37	110.36
1	B	5	THR	N-CA-C	-5.11	99.97	108.34
1	A	337	ARG	N-CA-C	-5.03	105.69	111.07
1	B	106	LYS	N-CA-C	-5.03	105.69	111.07
1	A	194	GLN	N-CA-C	-5.01	107.20	113.72

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	4340	0	4357	220	0
1	B	4365	0	4386	190	0
2	A	37	0	20	4	0
2	B	37	0	20	1	0
All	All	8779	0	8783	408	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 (408) 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:422:ARG:HA	1:B:426:MET:HE2	1.36	1.03
1:A:422:ARG:HA	1:A:426:MET:HE2	1.45	0.96
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.50	0.92
1:B:510:ARG:HG2	1:B:510:ARG:HH11	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:HB2	1:A:326:SER:HB2	1.60	0.83
1:A:192:GLY:HA3	1:A:316:ASN:OD1	1.78	0.82
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.44	0.81
1:B:175:LEU:HD21	1:B:253:ILE:HG12	1.62	0.81
1:B:327:ALA:O	1:B:331:GLU:HB3	1.81	0.80
1:B:470:SER:O	1:B:474:LEU:HG	1.82	0.79
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.63	0.79
1:A:496:PRO:HG2	1:A:499:VAL:HG23	1.63	0.79
1:B:381:VAL:HG11	1:B:474:LEU:HD22	1.66	0.77
1:B:48:ARG:HG2	1:B:159:LEU:HD13	1.67	0.77
1:B:336:LEU:HD12	1:B:356:PRO:HD3	1.66	0.76
1:B:550:TRP:HZ2	1:B:564:LEU:HD13	1.49	0.75
1:A:170:CYS:HA	1:A:173:MET:HE3	1.67	0.75
1:B:83:LEU:HB2	1:B:173:MET:HA	1.69	0.74
1:A:455:GLU:HB2	1:A:458:ASP:OD2	1.86	0.74
1:B:14:CYS:HB2	1:B:139:MET:SD	2.28	0.73
1:B:555:TYR:CG	1:B:560:ILE:HG13	2.22	0.73
1:A:321:VAL:HG21	1:A:365:SER:HB3	1.70	0.73
1:A:321:VAL:CG2	1:A:365:SER:HB3	2.19	0.72
1:A:466:LEU:HD21	1:A:551:PHE:HE2	1.53	0.72
1:B:527:ASN:HD21	1:B:534:LEU:HB2	1.53	0.72
1:B:461:GLN:HG3	1:B:539:ILE:HG21	1.71	0.70
1:B:231:ASN:O	1:B:235:VAL:HG23	1.90	0.70
1:A:94:PRO:HG3	1:A:109:ARG:CZ	2.22	0.70
1:A:501:ARG:NH1	2:A:5001:154:H26	2.07	0.69
1:A:20:LYS:H	1:A:20:LYS:HD2	1.58	0.69
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.22	0.69
1:B:555:TYR:CD1	1:B:560:ILE:HG13	2.27	0.69
1:B:141:LYS:HE3	1:B:160:ILE:HD13	1.75	0.69
1:B:41:THR:HG23	1:B:43:ARG:HB2	1.74	0.68
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.76	0.68
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.75	0.68
1:B:510:ARG:HG2	1:B:510:ARG:NH1	2.07	0.68
1:B:422:ARG:CA	1:B:426:MET:HE2	2.21	0.67
1:A:422:ARG:CA	1:A:426:MET:HE2	2.24	0.67
1:A:175:LEU:O	1:A:179:VAL:HG22	1.94	0.67
1:A:555:TYR:CG	1:A:560:ILE:HG13	2.30	0.67
1:A:510:ARG:HG2	1:A:510:ARG:HH11	1.59	0.67
1:B:52:VAL:HG12	1:B:223:CYS:SG	2.35	0.67
1:B:227:THR:HB	1:B:347:SER:O	1.96	0.66
1:A:82:LEU:HD12	1:A:173:MET:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:THR:HG23	1:B:43:ARG:H	1.60	0.66
1:B:385:THR:HG21	1:B:481:GLU:OE1	1.96	0.66
1:B:197:PRO:O	1:B:201:VAL:HG23	1.96	0.66
1:B:439:LEU:O	1:B:456:PRO:HB2	1.95	0.65
1:B:390:THR:HB	1:B:391:PRO:HD3	1.77	0.65
1:A:390:THR:HB	1:A:391:PRO:HD3	1.79	0.65
1:A:336:LEU:CD1	1:A:356:PRO:HD3	2.26	0.65
1:A:204:LEU:HD21	1:A:314:LEU:CD2	2.27	0.65
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.62	0.65
1:B:527:ASN:ND2	1:B:534:LEU:HB2	2.12	0.65
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.12	0.64
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.12	0.64
1:A:523:LYS:O	1:A:527:ASN:HB2	1.96	0.64
1:A:227:THR:HB	1:A:347:SER:O	1.98	0.63
1:A:434:LEU:HD13	1:A:510:ARG:HB3	1.78	0.63
1:B:550:TRP:CZ2	1:B:564:LEU:HD13	2.32	0.63
1:A:22:PRO:HG2	1:A:401:ARG:HG3	1.80	0.63
1:B:374:HIS:CE1	1:B:380:ARG:HG3	2.33	0.63
1:B:201:VAL:O	1:B:205:VAL:HG23	1.98	0.63
1:A:204:LEU:HD21	1:A:314:LEU:HD22	1.80	0.63
1:A:527:ASN:HD21	1:A:534:LEU:H	1.46	0.62
1:B:503:ARG:O	1:B:507:VAL:HG23	1.99	0.62
1:A:14:CYS:HB2	1:A:139:MET:SD	2.39	0.62
1:A:527:ASN:ND2	1:A:534:LEU:HB2	2.15	0.62
1:B:465:ARG:HG3	1:B:465:ARG:HH11	1.65	0.62
1:B:41:THR:CG2	1:B:43:ARG:HB2	2.30	0.61
1:A:466:LEU:CD2	1:A:551:PHE:HE2	2.13	0.60
1:A:187:MET:HE1	1:A:292:THR:HG22	1.82	0.60
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.42	0.60
1:B:496:PRO:HG2	1:B:499:VAL:HG23	1.82	0.60
1:B:372:VAL:HG23	1:B:381:VAL:O	2.00	0.60
1:B:170:CYS:HA	1:B:173:MET:HE3	1.84	0.60
1:A:452:TYR:OH	1:A:550:TRP:HA	2.01	0.60
1:B:56:ARG:N	1:B:56:ARG:HD3	2.17	0.60
1:B:488:CYS:O	1:B:492:LEU:HD13	2.02	0.60
1:A:217:PHE:CE1	1:A:322:VAL:HB	2.36	0.60
1:A:422:ARG:HA	1:A:426:MET:CE	2.27	0.60
1:B:485:VAL:O	1:B:489:LEU:HG	2.02	0.60
1:B:217:PHE:CE1	1:B:322:VAL:HB	2.36	0.59
1:B:455:GLU:HB2	1:B:458:ASP:OD2	2.02	0.59
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:SER:O	1:A:474:LEU:HG	2.03	0.59
1:A:478:SER:O	1:A:482:ILE:HG13	2.02	0.59
1:A:510:ARG:HG2	1:A:510:ARG:NH1	2.15	0.59
1:A:31:LEU:HD12	1:A:492:LEU:HD23	1.85	0.59
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.85	0.59
1:B:139:MET:O	1:B:160:ILE:HG22	2.02	0.59
1:A:129:ASP:O	1:A:259:ARG:NH1	2.35	0.59
1:A:215:MET:SD	1:A:215:MET:C	2.86	0.58
1:A:233:ILE:HD13	1:A:262:ILE:HA	1.86	0.58
1:A:104:GLY:O	1:A:108:VAL:HG23	2.04	0.57
1:A:515:GLY:HA2	1:A:519:ALA:HB2	1.86	0.57
1:A:187:MET:HE3	1:A:296:TYR:HB2	1.86	0.57
1:A:369:ASN:O	1:A:384:LEU:HD12	2.03	0.57
1:A:201:VAL:O	1:A:205:VAL:HG23	2.04	0.57
1:B:346:TYR:O	1:B:347:SER:HB3	2.04	0.57
1:B:398:GLU:HA	1:B:401:ARG:O	2.05	0.57
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.34	0.57
1:A:176:TYR:HE1	1:A:560:ILE:HD12	1.69	0.57
1:A:175:LEU:HD21	1:A:253:ILE:HG12	1.86	0.57
1:A:524:TYR:CD2	1:A:536:LEU:HG	2.40	0.57
1:B:147:VAL:HG12	1:B:154:ARG:HG2	1.87	0.57
1:B:434:LEU:HD13	1:B:510:ARG:HB3	1.87	0.57
1:A:19:SER:H	1:A:20:LYS:HZ2	1.53	0.56
1:A:179:VAL:HG12	1:A:289:CYS:CB	2.35	0.56
1:A:292:THR:OG1	1:A:317:GLY:HA2	2.04	0.56
1:B:123:TRP:HH2	1:B:174:ALA:HB2	1.69	0.56
1:B:369:ASN:O	1:B:384:LEU:HD12	2.05	0.56
1:B:48:ARG:CG	1:B:159:LEU:HD13	2.34	0.56
1:A:461:GLN:CG	1:A:539:ILE:HG21	2.35	0.56
1:B:197:PRO:HB2	1:B:467:HIS:HE1	1.71	0.56
1:A:499:VAL:O	1:A:503:ARG:HG3	2.05	0.56
1:A:340:THR:CG2	1:A:350:PRO:HG3	2.36	0.56
1:A:284:VAL:HG22	1:A:287:THR:OG1	2.06	0.56
1:B:374:HIS:HA	1:B:379:LYS:O	2.06	0.56
1:B:131:VAL:HG12	1:B:132:THR:N	2.21	0.56
1:A:501:ARG:NH1	1:A:505:ARG:NH2	2.53	0.55
1:B:309:GLN:O	1:B:324:CYS:HB2	2.06	0.55
1:A:31:LEU:C	1:A:31:LEU:HD23	2.30	0.55
1:A:45:ALA:O	1:A:49:GLN:HG3	2.07	0.55
1:B:97:ALA:O	1:B:165:LEU:HD22	2.06	0.55
1:B:440:GLU:HB3	1:B:457:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:GLU:OE2	1:A:280:ARG:NH2	2.37	0.55
1:A:416:ALA:HB3	1:A:417:PRO:HD3	1.89	0.55
1:A:217:PHE:CZ	1:A:322:VAL:HB	2.42	0.54
1:A:440:GLU:OE1	1:A:440:GLU:N	2.40	0.54
1:A:457:LEU:HB3	1:A:517:ARG:HB3	1.88	0.54
1:A:165:LEU:HD13	1:A:168:ARG:HH21	1.72	0.54
1:B:414:MET:HE2	1:B:447:ILE:HG23	1.88	0.54
1:B:196:SER:OG	1:B:199:GLN:HG3	2.08	0.53
1:B:233:ILE:HD13	1:B:262:ILE:HA	1.90	0.53
1:B:451:CYS:O	1:B:561:TYR:CD2	2.61	0.53
1:A:99:SER:C	1:A:101:PHE:H	2.15	0.53
1:A:123:TRP:CH2	1:A:174:ALA:HB2	2.43	0.53
1:B:249:ALA:O	1:B:253:ILE:HG13	2.08	0.53
1:B:368:SER:HA	1:B:386:ARG:HB3	1.90	0.53
1:A:202:GLU:HG2	1:A:206:ASN:ND2	2.24	0.53
1:A:359:ASP:HB3	1:A:362:LEU:HD12	1.89	0.53
1:A:83:LEU:CB	1:A:173:MET:HA	2.39	0.53
1:A:123:TRP:HH2	1:A:174:ALA:HB2	1.74	0.53
1:A:527:ASN:HD21	1:A:534:LEU:N	2.07	0.53
1:A:360:LEU:C	1:A:362:LEU:H	2.17	0.53
1:A:423:MET:HE1	2:A:5001:154:H21	1.90	0.53
1:B:423:MET:HE1	2:B:6001:154:H21	1.91	0.53
1:A:60:LEU:HD13	1:A:64:TYR:CE2	2.44	0.53
1:B:422:ARG:HA	1:B:426:MET:CE	2.23	0.53
1:A:175:LEU:HD13	1:A:286:THR:CG2	2.39	0.52
1:A:182:LEU:HD22	1:A:293:LEU:HD11	1.91	0.52
1:B:94:PRO:HD3	1:B:561:TYR:CD2	2.43	0.52
1:B:396:ALA:O	1:B:399:THR:HB	2.09	0.52
1:A:110:ASN:O	1:A:111:LEU:HB2	2.10	0.52
1:B:294:THR:HG22	1:B:298:LYS:HE3	1.91	0.52
1:B:93:PRO:HB2	1:B:96:SER:HB2	1.90	0.52
1:A:364:THR:HA	1:A:368:SER:O	2.11	0.51
1:A:464:GLU:OE2	1:A:469:LEU:HD21	2.10	0.51
1:A:48:ARG:CG	1:A:159:LEU:HD13	2.40	0.51
1:A:519:ALA:O	1:A:523:LYS:HB2	2.09	0.51
1:B:31:LEU:HG	1:B:492:LEU:HB3	1.90	0.51
1:B:235:VAL:O	1:B:239:ILE:HG13	2.10	0.51
1:A:197:PRO:HB2	1:A:467:HIS:HE1	1.75	0.51
1:B:38:TYR:CD2	1:B:154:ARG:HD2	2.46	0.51
1:A:504:ALA:HB1	1:A:526:PHE:CD1	2.46	0.51
1:B:14:CYS:SG	1:B:139:MET:HE1	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ALA:O	1:B:76:SER:HB2	2.11	0.51
1:B:84:SER:O	1:B:85:VAL:C	2.54	0.51
1:B:535:LYS:HG3	1:B:536:LEU:H	1.76	0.51
1:A:33:HIS:HB2	1:A:492:LEU:O	2.11	0.51
1:B:187:MET:HG2	1:B:296:TYR:CG	2.46	0.51
1:B:337:ARG:HB3	1:B:337:ARG:NH1	2.26	0.51
1:A:461:GLN:HG2	1:A:539:ILE:HG21	1.93	0.51
1:B:207:THR:HG22	1:B:323:ILE:HG21	1.93	0.51
1:A:30:LEU:O	1:A:494:VAL:HA	2.10	0.51
1:A:408:TRP:O	1:A:412:ILE:HG13	2.11	0.51
1:B:446:GLN:HE21	1:B:451:CYS:HB2	1.76	0.51
1:A:197:PRO:O	1:A:201:VAL:HG23	2.11	0.50
1:B:47:LEU:O	1:B:50:LYS:HB2	2.11	0.50
1:A:231:ASN:O	1:A:235:VAL:HG23	2.11	0.50
1:A:508:ARG:CZ	1:A:512:LEU:HD11	2.41	0.50
1:A:527:ASN:HD21	1:A:534:LEU:HB2	1.75	0.50
1:B:545:LEU:HB3	1:B:547:LEU:HD13	1.93	0.50
1:A:202:GLU:HG2	1:A:206:ASN:HD21	1.75	0.50
1:B:182:LEU:HB3	1:B:183:PRO:HD3	1.93	0.50
1:A:138:ILE:HG23	1:A:138:ILE:O	2.10	0.50
1:B:523:LYS:O	1:B:527:ASN:HB2	2.12	0.50
1:A:458:ASP:CG	1:A:517:ARG:HH22	2.20	0.50
1:B:298:LYS:NZ	1:B:346:TYR:O	2.42	0.50
1:B:236:GLU:OE2	1:B:280:ARG:NH2	2.39	0.50
1:A:7:THR:HG23	1:A:275:GLY:HA2	1.94	0.50
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.52	0.50
1:B:491:LYS:HG2	1:B:492:LEU:HD12	1.93	0.50
1:B:508:ARG:CZ	1:B:512:LEU:HD11	2.42	0.50
1:A:381:VAL:HG11	1:A:474:LEU:HD22	1.93	0.49
1:B:46:GLY:O	1:B:50:LYS:HD3	2.11	0.49
1:B:439:LEU:HD23	1:B:457:LEU:HD21	1.93	0.49
1:A:447:ILE:HB	1:A:452:TYR:HE2	1.77	0.49
1:A:237:GLU:HG3	1:A:257:THR:OG1	2.12	0.49
1:A:309:GLN:O	1:A:324:CYS:HB2	2.12	0.49
1:A:375:ASP:OD1	1:A:377:SER:N	2.44	0.49
1:B:239:ILE:O	1:B:242:CYS:HB2	2.12	0.49
1:A:59:VAL:HG13	1:B:59:VAL:HG13	1.94	0.49
1:A:179:VAL:HG12	1:A:289:CYS:HB3	1.95	0.49
1:A:83:LEU:HB2	1:A:173:MET:HA	1.95	0.49
1:A:175:LEU:HD12	1:A:261:TYR:OH	2.12	0.49
1:A:294:THR:CG2	1:A:298:LYS:HE3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:O	1:A:460:PRO:HD2	2.12	0.49
1:A:485:VAL:O	1:A:489:LEU:HG	2.12	0.49
1:B:337:ARG:CB	1:B:337:ARG:HH11	2.25	0.49
1:A:182:LEU:CD2	1:A:293:LEU:HD11	2.44	0.48
1:A:447:ILE:HG21	1:A:551:PHE:CE1	2.48	0.48
1:A:503:ARG:O	1:A:507:VAL:HG23	2.13	0.48
1:A:346:TYR:O	1:A:347:SER:HB3	2.12	0.48
1:B:187:MET:HE1	1:B:292:THR:HG22	1.96	0.48
1:B:419:LEU:HD22	1:B:482:ILE:HG12	1.95	0.48
1:A:526:PHE:C	1:A:528:TRP:H	2.21	0.48
1:B:141:LYS:CE	1:B:160:ILE:HD13	2.43	0.48
1:B:215:MET:SD	1:B:215:MET:C	2.97	0.48
1:A:414:MET:HE2	1:A:447:ILE:HG23	1.94	0.48
1:B:294:THR:O	1:B:298:LYS:HG3	2.14	0.48
1:B:234:ARG:NH1	1:B:258:GLU:OE2	2.39	0.48
1:B:561:TYR:CG	1:B:562:HIS:N	2.82	0.48
1:A:139:MET:O	1:A:160:ILE:HG22	2.13	0.48
1:A:24:ASN:ND2	1:A:400:ALA:HA	2.29	0.47
1:A:359:ASP:O	1:A:362:LEU:HB2	2.13	0.47
1:B:233:ILE:CD1	1:B:262:ILE:HA	2.43	0.47
1:B:340:THR:CG2	1:B:350:PRO:HG3	2.44	0.47
1:B:381:VAL:HG11	1:B:474:LEU:CD2	2.42	0.47
1:A:292:THR:OG1	1:A:317:GLY:N	2.46	0.47
1:A:88:ALA:HB1	1:A:169:VAL:HG13	1.96	0.47
1:A:183:PRO:HB2	1:A:191:TYR:CE2	2.49	0.47
1:A:523:LYS:HE2	1:A:534:LEU:HD23	1.96	0.47
1:A:19:SER:H	1:A:20:LYS:NZ	2.12	0.47
1:A:234:ARG:NH1	1:A:258:GLU:OE2	2.41	0.47
1:A:236:GLU:O	1:A:239:ILE:HB	2.15	0.47
1:B:38:TYR:CG	1:B:154:ARG:HD2	2.50	0.47
1:A:102:GLY:C	1:A:114:LYS:HE3	2.40	0.47
1:A:187:MET:HE1	1:A:292:THR:CG2	2.44	0.47
1:A:182:LEU:HB3	1:A:183:PRO:HD3	1.95	0.47
1:B:104:GLY:O	1:B:107:ASP:HB2	2.14	0.47
1:A:59:VAL:CG1	1:B:59:VAL:HG13	2.44	0.46
1:A:182:LEU:HD11	1:A:239:ILE:HG22	1.96	0.46
1:A:292:THR:OG1	1:A:317:GLY:CA	2.64	0.46
1:A:447:ILE:C	1:A:449:GLY:N	2.73	0.46
1:A:461:GLN:HG3	1:A:539:ILE:HG21	1.95	0.46
1:A:22:PRO:HG2	1:A:401:ARG:CG	2.43	0.46
1:A:161:VAL:O	1:A:283:GLY:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ALA:O	1:A:399:THR:HB	2.15	0.46
1:B:313:MET:HE3	1:B:313:MET:HB2	1.73	0.46
1:A:81:LYS:N	1:A:177:ASP:OD2	2.37	0.46
1:A:508:ARG:HE	1:A:530:VAL:HG11	1.81	0.46
1:B:123:TRP:CH2	1:B:174:ALA:HB2	2.50	0.46
1:B:388:PRO:HG2	1:B:488:CYS:SG	2.55	0.46
1:B:43:ARG:HG3	1:B:43:ARG:HH11	1.81	0.46
1:B:102:GLY:O	1:B:114:LYS:HE2	2.15	0.46
1:B:187:MET:HE1	1:B:292:THR:CG2	2.45	0.46
1:A:86:GLU:CD	1:A:86:GLU:H	2.23	0.46
1:A:204:LEU:HD21	1:A:314:LEU:HD23	1.98	0.46
1:A:399:THR:O	1:A:399:THR:HG22	2.16	0.46
1:B:428:HIS:HB2	1:B:500:TRP:CZ3	2.51	0.45
1:A:20:LYS:H	1:A:20:LYS:CD	2.24	0.45
1:A:89:CYS:HB3	1:A:108:VAL:O	2.16	0.45
1:A:412:ILE:HD13	1:A:426:MET:HG2	1.98	0.45
1:A:439:LEU:O	1:A:457:LEU:HG	2.17	0.45
1:B:26:LEU:HD13	1:B:432:ILE:HD13	1.97	0.45
1:A:59:VAL:HG13	1:B:59:VAL:CG1	2.46	0.45
1:A:96:SER:O	1:A:97:ALA:C	2.59	0.45
1:A:215:MET:HB2	1:A:326:SER:CB	2.39	0.45
1:B:161:VAL:O	1:B:283:GLY:N	2.42	0.45
1:B:96:SER:O	1:B:97:ALA:C	2.60	0.45
1:A:359:ASP:OD1	1:A:359:ASP:C	2.60	0.45
1:A:374:HIS:HA	1:A:379:LYS:O	2.16	0.45
1:B:273:ASN:ND2	1:B:275:GLY:H	2.14	0.45
1:B:419:LEU:CD2	1:B:482:ILE:HG12	2.47	0.45
1:B:464:GLU:OE2	1:B:538:PRO:HA	2.17	0.45
1:B:563:SER:O	1:B:565:SER:N	2.50	0.45
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.98	0.45
1:B:219:TYR:CZ	1:B:350:PRO:HB3	2.52	0.45
1:B:499:VAL:O	1:B:503:ARG:HG3	2.16	0.45
1:B:26:LEU:HD13	1:B:432:ILE:CD1	2.47	0.44
1:B:79:LYS:HA	1:B:244:ASP:HB3	1.99	0.44
1:B:489:LEU:HD22	1:B:494:VAL:HG11	1.98	0.44
1:A:466:LEU:CD2	1:A:551:PHE:CE2	2.98	0.44
1:B:138:ILE:HG23	1:B:138:ILE:O	2.16	0.44
1:B:464:GLU:OE2	1:B:469:LEU:HD21	2.17	0.44
1:A:408:TRP:HB2	1:A:429:PHE:CE2	2.53	0.44
1:A:539:ILE:HB	1:A:542:ALA:HB2	1.98	0.44
1:A:461:GLN:HB3	1:A:542:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:HG12	1:B:289:CYS:CB	2.47	0.44
1:B:492:LEU:HD12	1:B:492:LEU:N	2.32	0.44
1:B:204:LEU:HD21	1:B:314:LEU:CD2	2.48	0.44
1:A:465:ARG:HD3	1:A:542:ALA:O	2.16	0.44
1:B:81:LYS:HA	1:B:81:LYS:HE2	1.98	0.44
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.00	0.44
1:B:313:MET:HG2	1:B:322:VAL:HG22	1.99	0.44
1:B:377:SER:C	1:B:379:LYS:H	2.26	0.44
1:A:508:ARG:NE	1:A:530:VAL:HG11	2.33	0.44
1:B:422:ARG:NH2	1:B:472:PHE:O	2.51	0.44
1:B:441:LYS:O	1:B:443:LEU:HG	2.18	0.44
1:A:535:LYS:HG3	1:A:536:LEU:H	1.83	0.44
1:B:492:LEU:N	1:B:492:LEU:CD1	2.81	0.44
1:A:23:ILE:HG23	1:A:27:SER:CB	2.47	0.43
1:A:113:SER:O	1:A:117:ASN:ND2	2.52	0.43
1:B:160:ILE:O	1:B:160:ILE:HG23	2.17	0.43
1:B:179:VAL:HG12	1:B:289:CYS:SG	2.59	0.43
1:B:187:MET:HG2	1:B:296:TYR:CD2	2.53	0.43
1:B:52:VAL:HB	1:B:226:SER:OG	2.18	0.43
1:B:308:LEU:CD1	1:B:335:SER:HB3	2.48	0.43
1:B:337:ARG:HB3	1:B:337:ARG:HH11	1.83	0.43
1:B:372:VAL:CG2	1:B:373:ALA:N	2.81	0.43
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.53	0.43
1:B:175:LEU:HD12	1:B:261:TYR:OH	2.19	0.43
1:B:388:PRO:O	1:B:389:THR:C	2.59	0.43
1:A:125:ASP:O	1:A:129:ASP:HB3	2.19	0.43
1:A:172:LYS:CE	1:A:559:ASP:O	2.67	0.43
1:A:360:LEU:C	1:A:362:LEU:N	2.77	0.43
1:A:496:PRO:HG2	1:A:499:VAL:CG2	2.42	0.43
1:A:33:HIS:HB3	1:A:36:MET:CG	2.49	0.43
1:A:422:ARG:HD3	2:A:5001:154:CL14	2.55	0.43
1:A:510:ARG:O	1:A:514:GLN:HG2	2.18	0.43
1:B:517:ARG:HG2	1:B:517:ARG:HH11	1.84	0.43
1:A:30:LEU:O	1:A:494:VAL:HG13	2.18	0.43
1:A:87:GLU:O	1:A:88:ALA:C	2.62	0.43
1:B:94:PRO:HD3	1:B:561:TYR:CG	2.54	0.43
1:A:99:SER:C	1:A:101:PHE:N	2.75	0.43
1:A:368:SER:CB	1:A:384:LEU:HD11	2.49	0.43
1:A:526:PHE:C	1:A:528:TRP:N	2.76	0.43
1:A:526:PHE:HA	1:A:528:TRP:NE1	2.33	0.43
1:B:56:ARG:N	1:B:56:ARG:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ASP:O	1:A:459:LEU:C	2.60	0.43
1:B:440:GLU:OE1	1:B:440:GLU:N	2.50	0.43
1:A:160:ILE:O	1:A:160:ILE:HG23	2.19	0.42
1:A:372:VAL:HG22	1:A:373:ALA:N	2.34	0.42
1:A:504:ALA:HB1	1:A:526:PHE:HD1	1.83	0.42
1:B:406:ASN:ND2	1:B:443:LEU:HB3	2.33	0.42
1:A:235:VAL:O	1:A:236:GLU:C	2.62	0.42
1:A:326:SER:OG	1:A:332:ASP:OD2	2.37	0.42
1:A:235:VAL:O	1:A:239:ILE:HG13	2.19	0.42
1:A:71:MET:HE2	1:A:186:VAL:HG11	2.01	0.42
1:A:97:ALA:O	1:A:165:LEU:HD22	2.19	0.42
1:A:428:HIS:HB2	1:A:500:TRP:CZ3	2.55	0.42
1:B:447:ILE:C	1:B:449:GLY:N	2.77	0.42
1:A:175:LEU:O	1:A:176:TYR:C	2.63	0.42
1:A:375:ASP:OD1	1:A:375:ASP:C	2.62	0.42
1:B:176:TYR:HE1	1:B:560:ILE:HD12	1.84	0.42
1:B:561:TYR:CD1	1:B:562:HIS:N	2.88	0.42
1:A:79:LYS:O	1:A:79:LYS:HG2	2.20	0.42
1:B:82:LEU:HD12	1:B:173:MET:O	2.20	0.42
1:B:217:PHE:CZ	1:B:322:VAL:HB	2.54	0.42
1:B:540:PRO:C	1:B:542:ALA:H	2.27	0.42
1:A:320:LEU:HD12	1:A:321:VAL:H	1.85	0.42
1:B:523:LYS:HG3	1:B:534:LEU:CD2	2.50	0.42
1:B:539:ILE:O	1:B:542:ALA:HB3	2.19	0.42
1:A:92:THR:HA	1:A:93:PRO:HD3	1.93	0.41
2:A:5001:154:H162	2:A:5001:154:H231	1.72	0.41
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.59	0.41
1:A:385:THR:OG1	1:A:386:ARG:N	2.53	0.41
1:B:22:PRO:HG2	1:B:401:ARG:HG3	2.02	0.41
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.60	0.41
1:B:388:PRO:C	1:B:391:PRO:HD2	2.46	0.41
1:B:535:LYS:O	1:B:536:LEU:HB2	2.20	0.41
1:A:31:LEU:HG	1:A:492:LEU:HB3	2.00	0.41
1:A:203:PHE:CE2	1:A:314:LEU:HD13	2.54	0.41
1:A:414:MET:HE1	1:A:551:PHE:CE1	2.55	0.41
1:A:427:THR:HA	1:A:526:PHE:CZ	2.55	0.41
1:A:40:THR:O	1:A:142:ASN:HA	2.20	0.41
1:A:33:HIS:ND1	1:A:491:LYS:O	2.53	0.41
1:A:92:THR:HG21	1:A:165:LEU:HD11	2.03	0.41
1:A:207:THR:CG2	1:A:312:THR:HG21	2.50	0.41
1:A:361:GLU:HG2	1:A:370:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:PRO:O	1:A:389:THR:C	2.62	0.41
1:A:215:MET:CB	1:A:326:SER:HB2	2.41	0.41
1:B:545:LEU:HB3	1:B:547:LEU:CD1	2.50	0.41
1:A:340:THR:HG21	1:A:350:PRO:HG3	2.02	0.41
1:A:368:SER:HB2	1:A:384:LEU:HD11	2.03	0.41
1:B:118:HIS:O	1:B:121:SER:N	2.54	0.41
1:A:41:THR:OG1	1:A:43:ARG:HB2	2.21	0.41
1:A:132:THR:O	1:A:259:ARG:HB3	2.21	0.41
1:A:200:ARG:O	1:A:204:LEU:HG	2.20	0.41
1:A:243:CYS:HB2	1:A:245:LEU:HG	2.03	0.41
1:B:92:THR:HA	1:B:93:PRO:HD3	1.94	0.41
1:B:328:GLY:O	1:B:329:THR:C	2.64	0.41
1:B:434:LEU:HD21	1:B:511:LEU:HD23	2.03	0.41
1:A:389:THR:HA	1:A:488:CYS:SG	2.61	0.41
1:B:191:TYR:O	1:B:194:GLN:HG2	2.21	0.41
1:B:465:ARG:HH11	1:B:465:ARG:CG	2.33	0.41
1:A:387:ASP:OD1	1:A:387:ASP:C	2.64	0.40
1:B:172:LYS:NZ	1:B:559:ASP:HB3	2.36	0.40
1:B:200:ARG:HH21	1:B:365:SER:HB2	1.86	0.40
1:B:336:LEU:CD1	1:B:356:PRO:HD3	2.45	0.40
1:B:444:ASP:HB3	1:B:451:CYS:SG	2.61	0.40
1:A:43:ARG:HG3	1:A:43:ARG:HH11	1.85	0.40
1:A:123:TRP:HE3	1:A:170:CYS:SG	2.45	0.40
1:A:439:LEU:HG	1:A:457:LEU:CD2	2.52	0.40
1:B:184:GLN:C	1:B:184:GLN:CD	2.89	0.40
1:A:562:HIS:O	1:A:563:SER:C	2.64	0.40
1:B:215:MET:HE3	1:B:324:CYS:SG	2.62	0.40
1:B:386:ARG:NH2	1:B:391:PRO:HD3	2.37	0.40
1:A:310:ASP:O	1:A:324:CYS:HA	2.21	0.40
1:B:40:THR:O	1:B:142:ASN:HA	2.22	0.40
1:B:101:PHE:CD2	1:B:118:HIS:CE1	3.09	0.40
1:B:196:SER:O	1:B:197:PRO:C	2.64	0.40
1:B:510:ARG:NH1	1:B:510:ARG:CG	2.80	0.40
1:B:346:TYR:O	1:B:347:SER:CB	2.70	0.40
1:B:477:TYR:O	1:B:478:SER:C	2.65	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	554/578 (96%)	508 (92%)	44 (8%)	2 (0%)	30 59
1	B	557/578 (96%)	504 (90%)	47 (8%)	6 (1%)	11 36
All	All	1111/1156 (96%)	1012 (91%)	91 (8%)	8 (1%)	18 48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	85	VAL
1	A	90	LYS
1	B	564	LEU
1	A	536	LEU
1	B	97	ALA
1	B	536	LEU
1	B	90	LYS
1	B	540	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	476/492 (97%)	459 (96%)	17 (4%)	31 65
1	B	479/492 (97%)	460 (96%)	19 (4%)	28 62
All	All	955/984 (97%)	919 (96%)	36 (4%)	29 64

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

Mol	Chain	Res	Type
1	A	20	LYS
1	A	57	LEU
1	A	83	LEU
1	A	86	GLU
1	A	106	LYS
1	A	131	VAL
1	A	170	CYS
1	A	179	VAL
1	A	197	PRO
1	A	220	ASP
1	A	237	GLU
1	A	303	CYS
1	A	337	ARG
1	A	407	SER
1	A	440	GLU
1	A	510	ARG
1	A	534	LEU
1	B	14	CYS
1	B	20	LYS
1	B	47	LEU
1	B	57	LEU
1	B	86	GLU
1	B	120	HIS
1	B	131	VAL
1	B	262	ILE
1	B	303	CYS
1	B	308	LEU
1	B	321	VAL
1	B	355	GLN
1	B	366	CYS
1	B	377	SER
1	B	407	SER
1	B	440	GLU
1	B	466	LEU
1	B	510	ARG
1	B	534	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	206	ASN
1	A	273	ASN

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Mol	Chain	Res	Type
1	A	374	HIS
1	A	411	ASN
1	A	428	HIS
1	A	467	HIS
1	A	527	ASN
1	A	544	GLN
1	A	562	HIS
1	B	95	HIS
1	B	184	GLN
1	B	206	ASN
1	B	231	ASN
1	B	273	ASN
1	B	406	ASN
1	B	428	HIS
1	B	438	GLN
1	B	446	GLN
1	B	467	HIS
1	B	527	ASN
1	B	544	GLN
1	B	562	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 oligosaccharides 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	154	A	5001	-	41,41,41	2.39	19 (46%)	54,58,58	1.21	6 (11%)
2	154	B	6001	-	41,41,41	2.16	17 (41%)	54,58,58	1.21	7 (12%)

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	154	A	5001	-	-	13/28/28/28	0/5/5/5
2	154	B	6001	-	-	9/28/28/28	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	154	C23-N1	7.29	1.53	1.45
2	B	6001	154	C23-N1	5.74	1.51	1.45
2	A	5001	154	C2-N1	5.17	1.52	1.46
2	B	6001	154	C2-N1	4.54	1.51	1.46
2	B	6001	154	C6-N1	3.76	1.43	1.34
2	A	5001	154	C6-N1	3.69	1.43	1.34
2	B	6001	154	C8-C13	3.56	1.44	1.39
2	A	5001	154	C34-C33	3.38	1.45	1.38
2	B	6001	154	C34-C33	3.19	1.45	1.38
2	A	5001	154	C21-C22	2.93	1.43	1.38
2	A	5001	154	C22-C17	2.88	1.44	1.38
2	A	5001	154	C19-C18	2.80	1.43	1.38
2	A	5001	154	C8-C13	2.75	1.43	1.39
2	B	6001	154	C16-C2	2.73	1.59	1.54
2	A	5001	154	C31-C36	2.64	1.43	1.39
2	A	5001	154	C34-C35	2.63	1.43	1.38
2	A	5001	154	C10-C11	2.63	1.42	1.38
2	A	5001	154	C35-C36	2.62	1.45	1.39
2	A	5001	154	C18-C17	2.62	1.44	1.38
2	B	6001	154	C18-C17	2.57	1.44	1.38
2	B	6001	154	C22-C17	2.57	1.44	1.38
2	A	5001	154	C33-C32	2.51	1.43	1.38
2	B	6001	154	C19-C18	2.42	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5001	154	C12-C11	2.38	1.42	1.38
2	A	5001	154	C16-C2	2.38	1.58	1.54
2	B	6001	154	C33-C32	2.36	1.42	1.38
2	B	6001	154	C35-C36	2.34	1.44	1.39
2	B	6001	154	C12-C11	2.33	1.42	1.38
2	B	6001	154	C34-C35	2.32	1.42	1.38
2	B	6001	154	C12-C13	2.31	1.42	1.38
2	B	6001	154	C31-C36	2.29	1.42	1.39
2	A	5001	154	C12-C13	2.27	1.42	1.38
2	A	5001	154	C32-C31	2.26	1.45	1.41
2	B	6001	154	C21-C22	2.18	1.42	1.38
2	B	6001	154	C32-C31	2.11	1.44	1.41
2	A	5001	154	C20-C19	2.02	1.42	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	5001	154	C29-C27-S28	3.74	126.57	120.65
2	A	5001	154	C8-C6-N1	3.20	122.23	117.85
2	B	6001	154	C8-C6-N1	3.04	122.00	117.85
2	B	6001	154	C12-C13-C8	-2.90	119.22	121.59
2	B	6001	154	C29-C27-S28	2.67	124.89	120.65
2	B	6001	154	O7-C6-C8	-2.62	114.92	120.06
2	B	6001	154	C17-C16-C2	2.51	119.13	113.31
2	A	5001	154	C17-C16-C2	2.36	118.78	113.31
2	A	5001	154	O7-C6-C8	-2.32	115.50	120.06
2	B	6001	154	C23-N1-C6	2.29	123.22	116.95
2	A	5001	154	C26-C27-C29	-2.28	122.36	128.63
2	A	5001	154	C23-N1-C6	2.09	122.66	116.95
2	B	6001	154	C33-C32-C31	-2.04	117.86	120.95

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	154	C16-C2-N1-C23
2	B	6001	154	C2-C16-C17-C22
2	B	6001	154	C2-C16-C17-C18
2	A	5001	154	C2-C16-C17-C22
2	A	5001	154	C2-C16-C17-C18
2	A	5001	154	C26-C27-C29-O37
2	A	5001	154	S28-C27-C29-O37

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Mol	Chain	Res	Type	Atoms
2	B	6001	154	C26-C27-C29-O37
2	B	6001	154	S28-C27-C29-O37
2	A	5001	154	O7-C6-N1-C23
2	B	6001	154	N1-C23-C24-S28
2	B	6001	154	N1-C23-C24-C25
2	A	5001	154	N1-C23-C24-S28
2	A	5001	154	C26-C27-C29-C30
2	A	5001	154	S28-C27-C29-C30
2	B	6001	154	C26-C27-C29-C30
2	B	6001	154	S28-C27-C29-C30
2	A	5001	154	N1-C23-C24-C25
2	A	5001	154	N1-C2-C3-O5
2	A	5001	154	C8-C6-N1-C23
2	B	6001	154	C16-C2-N1-C23
2	A	5001	154	C16-C2-C3-O5

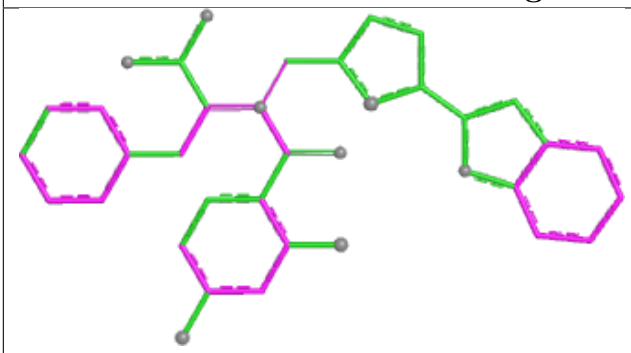
There are no ring outliers.

2 monomers are involved in 5 short contacts:

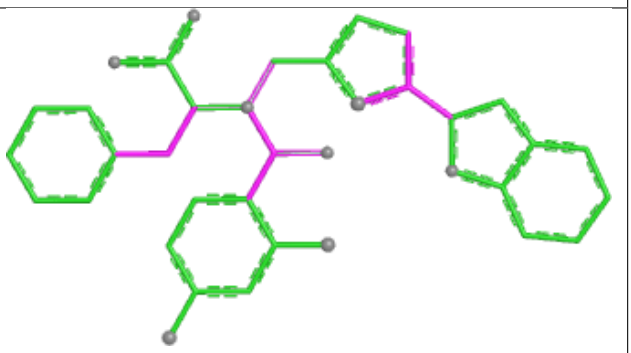
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	154	4	0
2	B	6001	154	1	0

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.

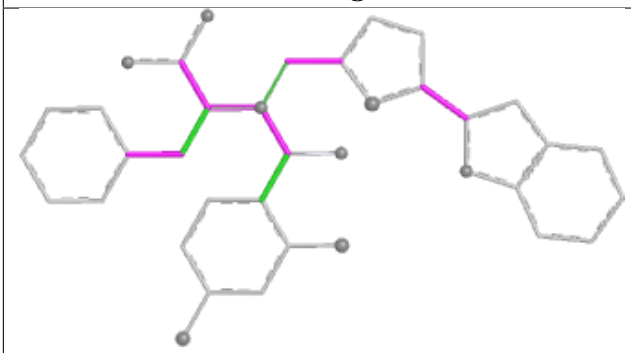
Ligand 154 A 5001



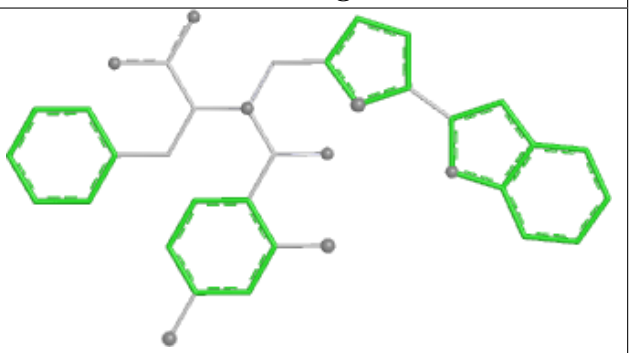
Bond lengths



Bond angles

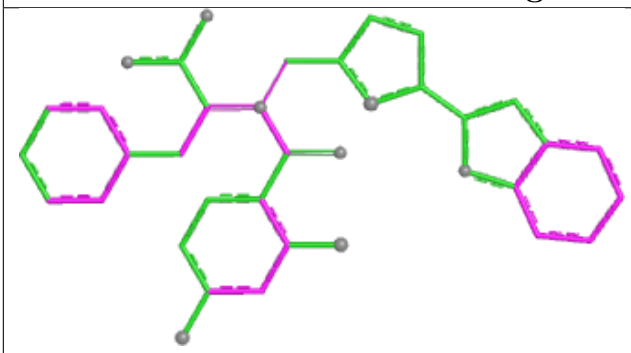


Torsions

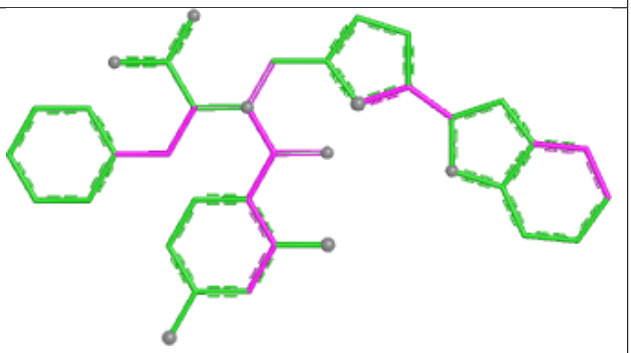


Rings

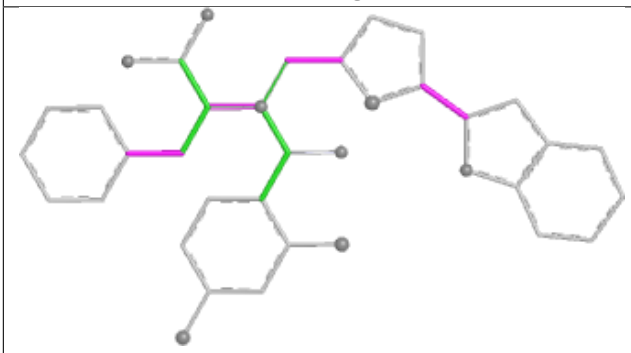
Ligand 154 B 6001



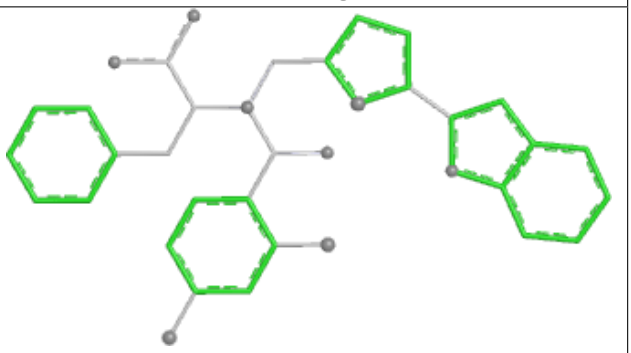
Bond lengths



Bond angles



Torsions



Rings

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

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	558/578 (96%)	0.35	37 (6%)	24	19	8, 28, 63, 102	0
1	B	561/578 (97%)	0.40	38 (6%)	23	18	9, 29, 70, 99	0
All	All	1119/1156 (96%)	0.38	75 (6%)	24	19	8, 28, 68, 102	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	556	SER	6.4
1	B	561	TYR	6.2
1	B	550	TRP	6.1
1	A	550	TRP	5.9
1	B	556	SER	5.8
1	B	549	GLY	5.7
1	A	560	ILE	5.6
1	B	563	SER	5.4
1	A	547	LEU	5.4
1	B	552	VAL	5.3
1	A	559	ASP	5.0
1	A	561	TYR	4.7
1	B	447	ILE	4.7
1	A	549	GLY	4.7
1	A	448	TYR	4.5
1	A	562	HIS	4.4
1	B	545	LEU	4.4
1	B	555	TYR	4.3
1	B	560	ILE	4.3
1	B	554	GLY	4.3
1	B	564	LEU	4.2
1	A	552	VAL	4.1
1	B	542	ALA	4.1
1	B	548	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	558	GLY	4.1
1	B	553	ALA	4.0
1	B	559	ASP	3.9
1	A	555	TYR	3.9
1	B	547	LEU	3.8
1	A	545	LEU	3.8
1	A	553	ALA	3.7
1	B	551	PHE	3.7
1	A	447	ILE	3.7
1	A	563	SER	3.7
1	B	541	ALA	3.5
1	A	544	GLN	3.5
1	A	546	ASP	3.3
1	B	562	HIS	3.3
1	B	566	ARG	3.3
1	B	565	SER	3.2
1	A	554	GLY	3.2
1	A	531	LYS	3.1
1	A	15	ALA	3.1
1	A	223	CYS	3.1
1	A	548	SER	3.0
1	B	544	GLN	3.0
1	B	538	PRO	2.9
1	A	535	LYS	2.9
1	A	95	HIS	2.8
1	B	543	SER	2.8
1	B	448	TYR	2.7
1	B	329	THR	2.7
1	A	536	LEU	2.6
1	B	540	PRO	2.6
1	B	546	ASP	2.6
1	B	557	GLY	2.5
1	A	551	PHE	2.5
1	A	543	SER	2.5
1	A	540	PRO	2.4
1	A	558	GLY	2.4
1	A	557	GLY	2.4
1	B	446	GLN	2.4
1	B	95	HIS	2.3
1	A	542	ALA	2.3
1	B	1	SER	2.3
1	A	451	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	93	PRO	2.2
1	B	450	ALA	2.2
1	B	445	CYS	2.2
1	A	446	GLN	2.2
1	A	450	ALA	2.2
1	B	535	LYS	2.1
1	B	536	LEU	2.0
1	A	449	GLY	2.0
1	A	106	LYS	2.0

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 oligosaccharides in this entry.

6.4 Ligands (i)

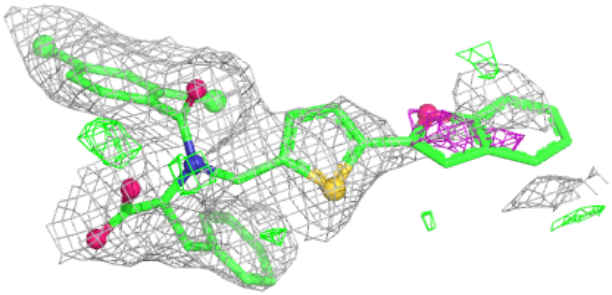
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

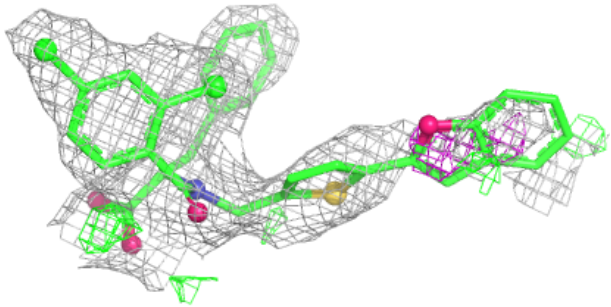
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	154	A	5001	37/37	0.78	0.17	37,44,58,59	0
2	154	B	6001	37/37	0.79	0.16	40,46,61,61	0

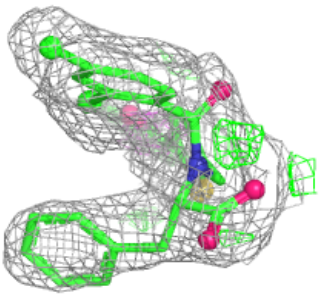
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 154 A 5001:

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

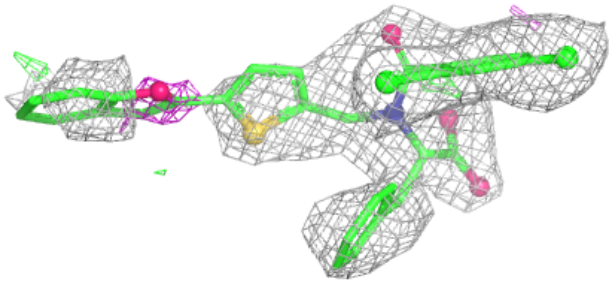


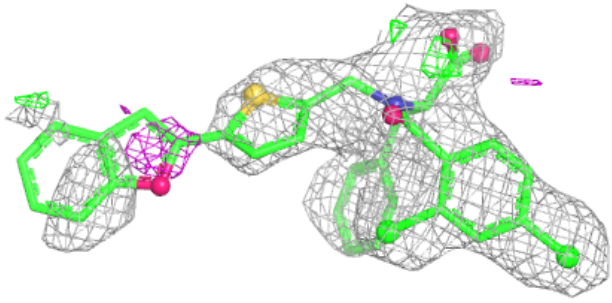


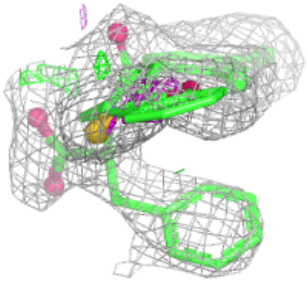


Electron density around 154 B 6001:

$2mF_o$-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.