



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:41 PM UTC

PDB ID : 4JH0 / pdb_00004jh0
Title : Crystal structure of dipeptidyl-peptidase 4 (CD26, adenosine deaminase complexing protein 2) (DPP-IV-WT) complex with bms-767778 AKA 2-(3-(aminomethyl)-4-(2,4-dichlorophenyl)-2-methyl-5-oxo-5,7-dihydro-6h-pyrrolo[3,4-b]pyridin-6-yl)-n,n-dimethylacetamide
Authors : Klei, H.E.
Deposited on : 2013-03-04
Resolution : 2.35 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

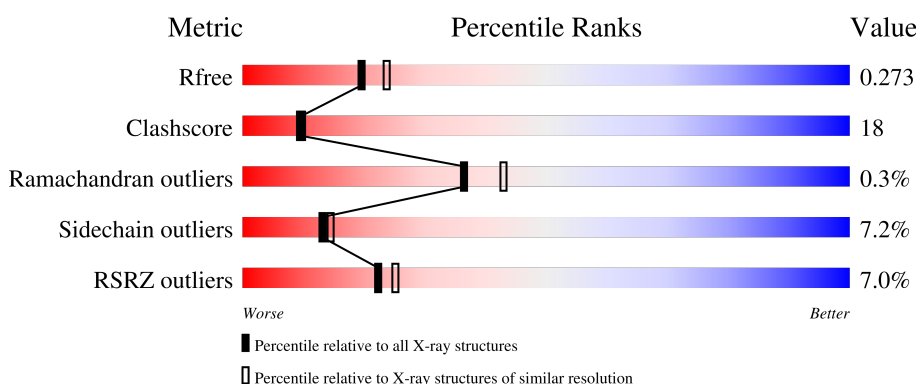
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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 $\leq 5\%$. 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	728	6% 66% 30% 5%
1	B	728	8% 67% 28% .

2 Entry composition [i](#)

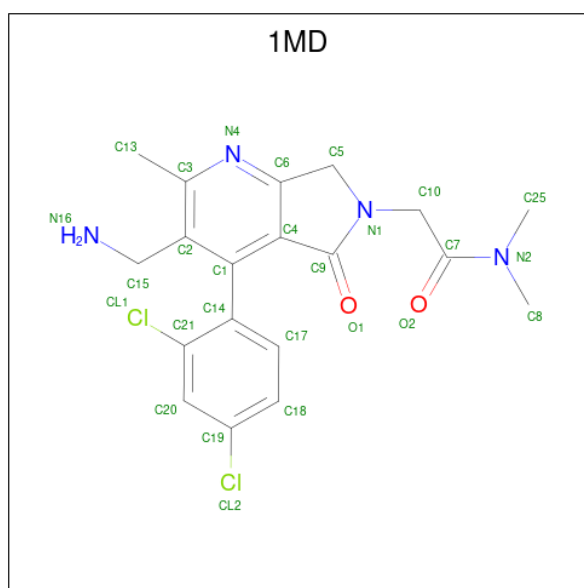
There are 3 unique types of molecules in this entry. The entry contains 12054 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is 2-[3-(aminomethyl)-4-(2,4-dichlorophenyl)-2-methyl-5-oxo-5,7-dihydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-N,N-dimethylacetamide (CCD ID: 1MD) (formula: $C_{19}H_{20}Cl_2N_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	19	2	4	2		
2	B	1	Total	C	Cl	N	O	0	0
			27	19	2	4	2		

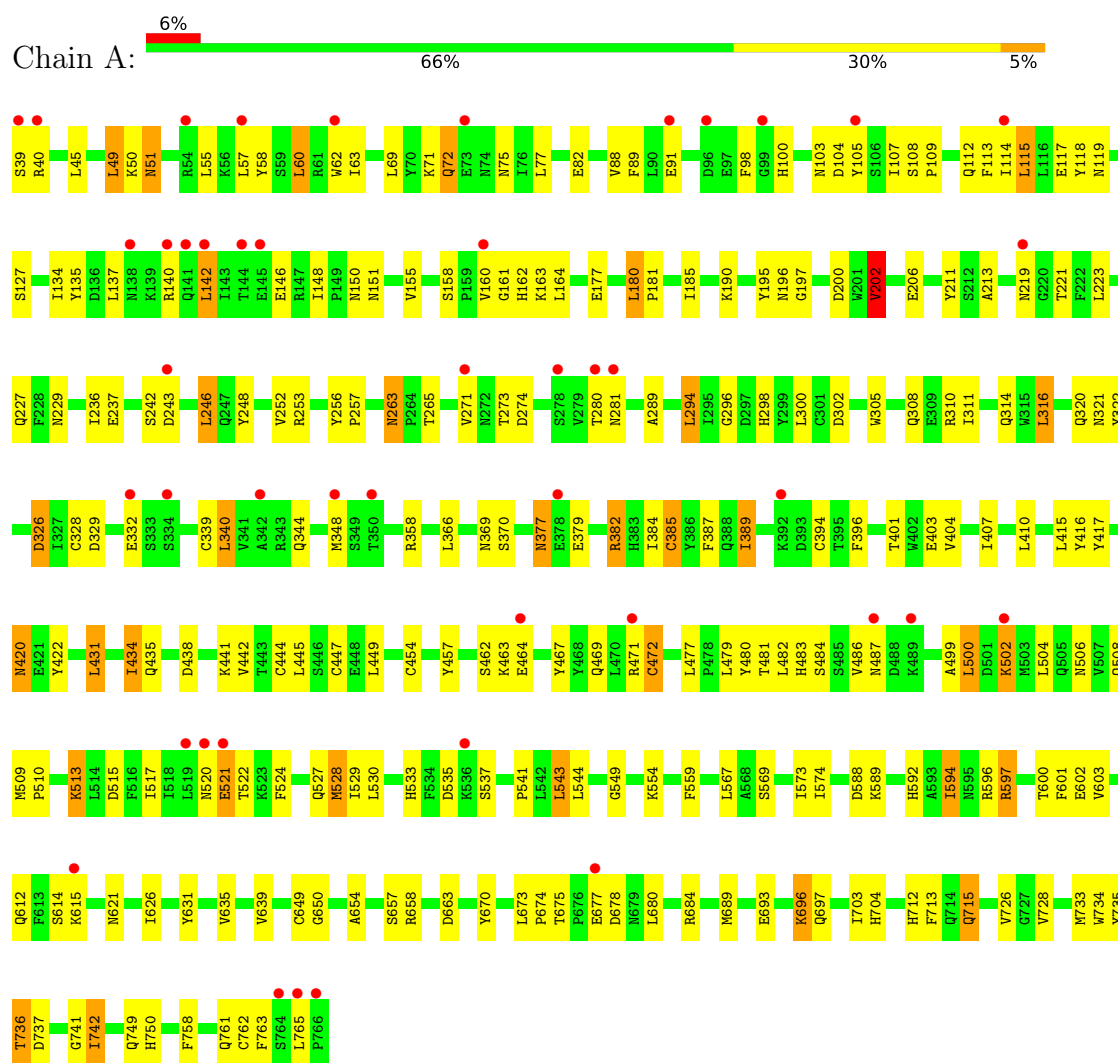
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total 34	O 34	0	0
3	B	40	Total 40	O 40	0	0

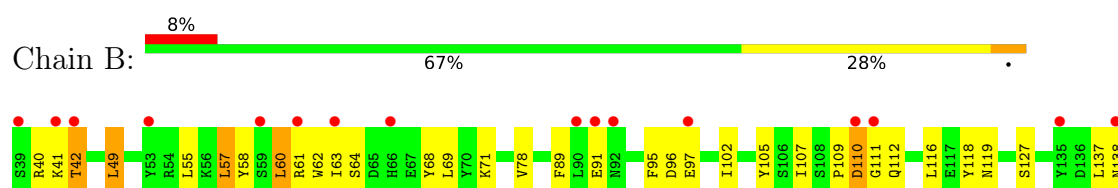
3 Residue-property plots

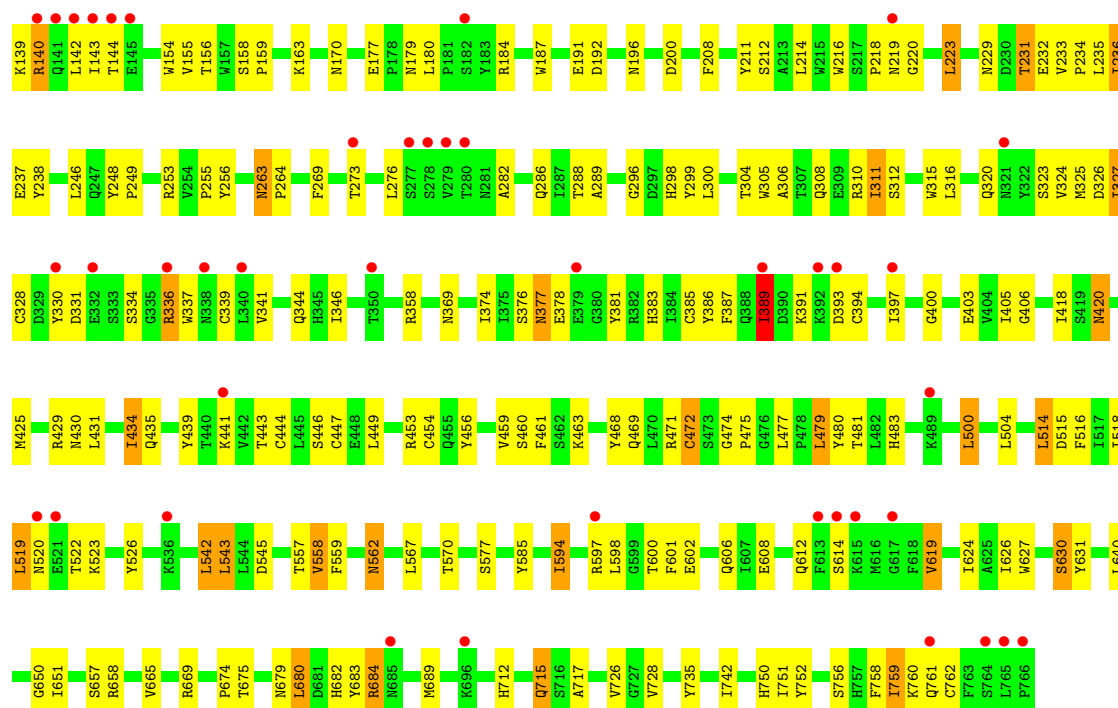
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.31Å 67.11Å 423.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.95 – 2.35 47.95 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.7 (47.95-2.35) 91.8 (47.95-2.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.34Å)	Xtriage
Refinement program	CNS, CNX 2005	Depositor
R, R_{free}	0.243 , 0.272 0.242 , 0.273	Depositor DCC
R_{free} test set	1546 reflections (2.13%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.075 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12054	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 1MD

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	0.44	0/6135	0.79	6/8344 (0.1%)
1	B	0.43	0/6135	0.79	6/8344 (0.1%)
All	All	0.44	0/12270	0.79	12/16688 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	389	ILE	N-CA-C	6.59	118.14	110.62
1	B	96	ASP	N-CA-C	-5.98	105.69	112.87
1	B	220	GLY	N-CA-C	-5.84	107.04	115.27
1	B	233	VAL	CA-C-N	5.75	125.70	119.78
1	B	233	VAL	C-N-CA	5.75	125.70	119.78
1	A	673	LEU	CA-C-N	5.66	126.92	119.84
1	A	673	LEU	C-N-CA	5.66	126.92	119.84
1	A	675	THR	CA-C-N	5.50	125.32	119.28
1	A	675	THR	C-N-CA	5.50	125.32	119.28
1	A	202	VAL	CB-CA-C	-5.44	104.79	112.14
1	B	389	ILE	N-CA-C	5.33	115.47	110.30
1	B	630	SER	CB-CA-C	-5.27	110.51	116.63

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	ASP	Peptide

5.2 Too-close contacts

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	5963	0	5695	216	0
1	B	5963	0	5695	196	0
2	A	27	0	20	0	0
2	B	27	0	20	0	0
3	A	34	0	0	6	0
3	B	40	0	0	9	0
All	All	12054	0	11430	402	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 18.

All (402) 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:340:LEU:H	1:A:340:LEU:HD12	1.25	0.99
1:A:434:ILE:HD13	1:A:434:ILE:H	1.35	0.92
1:A:658:ARG:NH2	1:A:684:ARG:HE	1.71	0.88
1:B:328:CYS:HG	1:B:339:CYS:HG	1.12	0.88
1:A:454:CYS:HG	1:A:472:CYS:HG	1.00	0.86
1:A:431:LEU:HD13	1:A:445:LEU:HD12	1.58	0.86
1:B:403:GLU:H	1:B:420:ASN:HD21	1.26	0.83
1:A:253:ARG:HH22	1:B:253:ARG:NH1	1.80	0.80
1:A:377:ASN:C	1:A:377:ASN:HD22	1.90	0.80
1:A:649:CYS:HG	1:A:762:CYS:HG	0.81	0.79
1:B:163:LYS:HD3	1:B:273:THR:HG21	1.63	0.78
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.84	0.78
1:A:597:ARG:HD3	1:A:600:THR:HG21	1.65	0.78
1:A:444:CYS:HG	1:A:447:CYS:HG	0.77	0.77
1:A:434:ILE:HG22	1:A:442:VAL:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:GLU:O	1:A:696:LYS:HG3	1.85	0.76
1:B:331:ASP:HB3	1:B:334:SER:HB3	1.68	0.76
1:A:567:LEU:HD22	1:A:573:ILE:HD12	1.65	0.76
1:A:415:LEU:HB3	1:A:434:ILE:HD11	1.67	0.74
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.51	0.73
1:A:508:GLN:HE21	1:A:533:HIS:HE1	1.37	0.72
1:B:562:ASN:C	1:B:562:ASN:HD22	1.95	0.72
1:A:658:ARG:HH21	1:A:684:ARG:HE	1.38	0.72
1:B:325:MET:HE2	1:B:327:ILE:HD11	1.71	0.72
1:B:726:VAL:HG13	1:B:728:VAL:HG23	1.71	0.71
1:A:177:GLU:HB2	1:A:180:LEU:HB2	1.72	0.70
1:A:750:HIS:HE1	1:B:728:VAL:O	1.75	0.70
1:A:734:TRP:HE1	1:A:736:THR:HG22	1.57	0.69
1:B:139:LYS:O	1:B:140:ARG:HG3	1.91	0.69
1:A:385:CYS:HG	1:A:394:CYS:HG	1.39	0.69
1:A:735:TYR:OH	1:A:750:HIS:HD2	1.76	0.69
1:A:734:TRP:NE1	1:A:736:THR:HG22	2.08	0.69
1:B:377:ASN:C	1:B:377:ASN:HD22	1.97	0.69
1:A:508:GLN:HE21	1:A:533:HIS:CE1	2.11	0.69
1:B:312:SER:HB2	1:B:325:MET:HE3	1.73	0.68
1:A:221:THR:O	1:A:273:THR:HB	1.94	0.68
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.77	0.67
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.75	0.67
1:A:658:ARG:NH2	1:A:684:ARG:NE	2.40	0.67
1:A:736:THR:HG21	1:B:717:ALA:O	1.96	0.66
1:B:137:LEU:C	1:B:139:LYS:H	2.04	0.66
1:A:696:LYS:HD2	1:A:697:GLN:HG3	1.79	0.65
1:B:159:PRO:HB2	3:B:929:HOH:O	1.96	0.65
1:A:736:THR:O	1:A:737:ASP:HB2	1.95	0.65
1:B:420:ASN:HD22	1:B:420:ASN:C	2.04	0.65
1:A:280:THR:HG22	1:A:281:ASN:O	1.95	0.65
1:A:55:LEU:HD21	1:A:559:PHE:HE2	1.60	0.64
1:B:110:ASP:HB2	3:B:904:HOH:O	1.96	0.64
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.31	0.64
1:A:328:CYS:HG	1:A:339:CYS:HG	0.64	0.64
1:B:218:PRO:HA	3:B:929:HOH:O	1.97	0.64
1:A:340:LEU:H	1:A:340:LEU:CD1	2.05	0.63
1:A:403:GLU:H	1:A:420:ASN:HD21	1.45	0.63
1:A:657:SER:H	1:A:715:GLN:NE2	1.96	0.63
1:B:543:LEU:HD21	1:B:627:TRP:HD1	1.61	0.63
1:A:358:ARG:NH1	1:A:358:ARG:HB3	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:THR:HG22	1:B:232:GLU:HG2	1.80	0.63
1:A:734:TRP:CD1	1:A:736:THR:HG22	2.33	0.63
1:A:40:ARG:HE	1:A:40:ARG:HA	1.65	0.62
1:B:658:ARG:HB2	1:B:689:MET:HE1	1.80	0.62
1:A:206:GLU:OE1	1:A:206:GLU:HA	2.00	0.62
1:A:305:TRP:CZ3	1:A:311:ILE:HG12	2.35	0.62
1:B:657:SER:H	1:B:715:GLN:NE2	1.98	0.62
1:B:477:LEU:HD22	1:B:500:LEU:HD13	1.82	0.62
1:A:758:PHE:O	1:A:761:GLN:HG3	2.00	0.61
1:B:435:GLN:HE22	1:B:441:LYS:HD2	1.64	0.61
1:B:453:ARG:O	1:B:475:PRO:HD2	1.99	0.61
1:A:219:ASN:HB2	1:A:308:GLN:OE1	2.00	0.61
1:A:340:LEU:HD12	1:A:340:LEU:N	2.08	0.61
1:B:459:VAL:HG22	1:B:460:SER:N	2.16	0.61
1:A:289:ALA:HB3	1:A:294:LEU:HD13	1.83	0.61
1:A:658:ARG:HH21	1:A:684:ARG:NE	1.97	0.61
1:A:658:ARG:HB2	1:A:689:MET:HE1	1.82	0.60
1:A:382:ARG:H	1:A:403:GLU:HG2	1.67	0.60
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.83	0.60
1:A:471:ARG:HG3	1:A:480:TYR:CE2	2.36	0.60
1:A:635:VAL:O	1:A:639:VAL:HG23	2.02	0.60
1:B:726:VAL:HG22	1:B:726:VAL:O	2.00	0.60
1:B:63:ILE:HD11	1:B:69:LEU:HD12	1.84	0.59
1:B:369:ASN:O	1:B:389:ILE:HG12	2.03	0.59
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.37	0.59
1:B:386:TYR:HB2	1:B:397:ILE:HD11	1.85	0.58
1:B:403:GLU:H	1:B:420:ASN:ND2	1.97	0.58
1:A:508:GLN:NE2	1:A:533:HIS:HE1	2.01	0.58
1:A:316:LEU:HD22	1:A:320:GLN:HG2	1.86	0.58
1:B:562:ASN:C	1:B:562:ASN:ND2	2.62	0.58
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.85	0.57
1:A:529:ILE:HD12	1:A:529:ILE:N	2.19	0.57
1:B:111:GLY:O	1:B:137:LEU:HD12	2.05	0.57
1:A:358:ARG:HB3	1:A:358:ARG:HH11	1.70	0.57
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.87	0.57
1:A:142:LEU:HD12	1:A:142:LEU:H	1.70	0.57
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.87	0.57
1:B:341:VAL:HG13	1:B:344:GLN:NE2	2.20	0.57
1:A:434:ILE:HD13	1:A:434:ILE:N	2.13	0.56
1:A:499:ALA:O	1:A:502:LYS:HG3	2.05	0.56
1:A:741:GLY:O	1:A:742:ILE:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLU:OE2	1:B:253:ARG:HD3	2.05	0.56
1:A:40:ARG:HA	1:A:40:ARG:NE	2.21	0.56
1:A:696:LYS:HB3	1:A:728:VAL:HG22	1.88	0.56
1:A:384:ILE:HG13	1:A:404:VAL:HG21	1.88	0.56
1:B:680:LEU:HD13	1:B:680:LEU:C	2.31	0.55
1:A:520:ASN:O	1:A:521:GLU:HG3	2.07	0.55
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.87	0.55
1:B:288:THR:HG22	1:B:289:ALA:O	2.06	0.55
1:A:370:SER:HB2	1:A:387:PHE:O	2.07	0.55
1:B:42:THR:HG23	1:B:570:THR:OG1	2.06	0.55
1:B:42:THR:CG2	1:B:570:THR:OG1	2.55	0.55
1:B:474:GLY:HA3	1:B:558:VAL:HA	1.88	0.55
1:A:477:LEU:HD22	1:A:500:LEU:HD13	1.87	0.55
1:B:377:ASN:C	1:B:377:ASN:ND2	2.65	0.54
1:A:596:ARG:HA	1:A:670:TYR:O	2.07	0.54
1:A:60:LEU:HD13	1:A:60:LEU:H	1.71	0.54
1:B:675:THR:C	1:B:680:LEU:HB2	2.33	0.54
1:B:142:LEU:HD12	1:B:142:LEU:H	1.72	0.54
1:B:500:LEU:CD2	1:B:504:LEU:HG	2.38	0.54
1:B:518:ILE:O	1:B:519:LEU:HD13	2.08	0.54
1:A:326:ASP:OD1	1:A:344:GLN:HG2	2.08	0.54
1:B:179:ASN:OD1	1:B:180:LEU:HD13	2.06	0.54
1:A:163:LYS:HZ2	1:A:273:THR:HG21	1.73	0.54
1:A:486:VAL:HG23	1:A:487:ASN:N	2.22	0.54
1:B:542:LEU:HD23	1:B:624:ILE:HG23	1.90	0.54
1:A:434:ILE:H	1:A:434:ILE:CD1	2.14	0.53
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.22	0.53
1:A:387:PHE:CD2	1:A:394:CYS:HB3	2.43	0.53
1:A:253:ARG:HH12	1:B:253:ARG:HH12	1.56	0.53
1:B:57:LEU:N	1:B:57:LEU:HD12	2.24	0.53
1:A:296:GLY:O	1:A:298:HIS:HD2	1.92	0.53
1:A:377:ASN:ND2	1:A:379:GLU:H	2.07	0.53
1:A:602:GLU:HG2	1:A:603:VAL:N	2.24	0.53
1:A:195:TYR:O	1:A:227:GLN:HA	2.09	0.53
1:A:253:ARG:HH22	1:B:253:ARG:HH12	1.57	0.53
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.91	0.53
1:A:60:LEU:HD13	1:A:60:LEU:N	2.24	0.52
1:A:60:LEU:O	1:A:60:LEU:HD22	2.08	0.52
1:B:127:SER:HA	1:B:211:TYR:CD2	2.44	0.52
1:B:296:GLY:O	1:B:298:HIS:HD2	1.93	0.52
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:ILE:C	1:B:434:ILE:HD13	2.34	0.52
1:A:55:LEU:HD23	1:A:500:LEU:CD1	2.39	0.52
1:B:429:ARG:NE	3:B:911:HOH:O	2.43	0.52
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.45	0.52
1:A:146:GLU:OE2	1:A:181:PRO:HG3	2.09	0.52
1:B:518:ILE:C	1:B:519:LEU:HD13	2.35	0.52
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.39	0.52
1:B:55:LEU:HD23	1:B:500:LEU:HD12	1.92	0.52
1:B:516:PHE:CE1	1:B:523:LYS:HE2	2.46	0.51
1:A:486:VAL:HG23	1:A:487:ASN:H	1.76	0.51
1:B:300:LEU:C	1:B:300:LEU:HD13	2.35	0.51
1:B:377:ASN:HD21	1:B:381:TYR:H	1.58	0.51
1:B:600:THR:OG1	1:B:601:PHE:N	2.43	0.51
1:A:58:TYR:HD1	1:A:60:LEU:HD12	1.76	0.51
1:A:221:THR:HG23	1:A:274:ASP:OD2	2.10	0.51
1:B:331:ASP:CB	1:B:334:SER:HB3	2.39	0.51
1:A:535:ASP:OD1	1:A:537:SER:HB3	2.09	0.51
1:B:418:ILE:HD13	1:B:431:LEU:HA	1.92	0.51
1:A:726:VAL:O	1:A:726:VAL:HG22	2.11	0.51
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.94	0.51
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.11	0.51
1:A:253:ARG:HH22	1:B:253:ARG:HH11	1.54	0.51
1:A:420:ASN:C	1:A:420:ASN:HD22	2.18	0.51
1:B:137:LEU:C	1:B:139:LYS:N	2.68	0.50
1:B:95:PHE:C	1:B:97:GLU:H	2.19	0.50
1:B:219:ASN:ND2	3:B:934:HOH:O	2.44	0.50
1:B:751:ILE:HG23	1:B:752:TYR:N	2.25	0.50
1:A:89:PHE:HE2	1:A:107:ILE:CD1	2.21	0.50
1:A:242:SER:OG	1:A:243:ASP:N	2.44	0.50
1:B:453:ARG:C	1:B:475:PRO:HD2	2.37	0.50
1:A:377:ASN:C	1:A:377:ASN:ND2	2.58	0.50
1:B:219:ASN:N	1:B:308:GLN:OE1	2.42	0.50
1:B:341:VAL:HA	1:B:344:GLN:HG3	1.94	0.50
1:B:459:VAL:HG22	1:B:460:SER:H	1.75	0.50
1:A:50:LYS:O	1:A:51:ASN:HB2	2.12	0.49
1:A:88:VAL:HG21	1:A:91:GLU:HG3	1.94	0.49
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.93	0.49
1:B:597:ARG:HA	1:B:682:HIS:CE1	2.47	0.49
1:A:221:THR:HG23	1:A:274:ASP:CG	2.36	0.49
1:A:369:ASN:O	1:A:389:ILE:HG12	2.12	0.49
1:B:640:LEU:HD11	1:B:650:GLY:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LEU:CD1	1:A:445:LEU:HD12	2.37	0.49
1:A:454:CYS:CB	1:A:472:CYS:HG	2.24	0.49
1:B:434:ILE:HG23	1:B:434:ILE:O	2.12	0.49
1:B:200:ASP:OD2	1:B:264:PRO:HG3	2.13	0.49
1:A:71:LYS:O	1:A:71:LYS:HG3	2.11	0.49
1:A:109:PRO:CB	1:A:160:VAL:HA	2.42	0.49
1:A:517:ILE:HD12	1:A:612:GLN:HG3	1.95	0.49
1:A:734:TRP:HE1	1:A:736:THR:CG2	2.25	0.49
1:B:756:SER:O	1:B:760:LYS:HG3	2.12	0.49
1:B:58:TYR:HD1	1:B:60:LEU:HD12	1.77	0.49
1:B:657:SER:H	1:B:715:GLN:HE21	1.60	0.49
1:A:543:LEU:HD12	1:A:567:LEU:CD1	2.43	0.48
1:A:112:GLN:O	1:A:137:LEU:HB2	2.13	0.48
1:B:229:ASN:ND2	3:B:901:HOH:O	2.39	0.48
1:B:434:ILE:HD11	1:B:439:TYR:HA	1.95	0.48
1:A:457:TYR:HA	1:A:471:ARG:O	2.14	0.48
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.96	0.48
1:A:522:THR:N	3:A:931:HOH:O	2.43	0.48
1:A:529:ILE:N	1:A:529:ILE:CD1	2.76	0.48
1:B:627:TRP:HA	1:B:651:ILE:O	2.13	0.48
1:B:236:ILE:HD12	1:B:712:HIS:CD2	2.49	0.48
1:B:155:VAL:O	1:B:156:THR:HG23	2.13	0.48
1:B:191:GLU:O	1:B:192:ASP:HB2	2.13	0.48
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.49	0.47
1:A:109:PRO:HD2	1:A:161:GLY:O	2.14	0.47
1:B:299:TYR:CZ	1:B:665:VAL:HG22	2.49	0.47
1:A:160:VAL:HG22	1:A:161:GLY:N	2.29	0.47
1:B:177:GLU:CB	1:B:180:LEU:HD22	2.44	0.47
1:A:596:ARG:N	1:A:670:TYR:O	2.47	0.47
1:A:55:LEU:HD23	1:A:500:LEU:HD12	1.95	0.47
1:A:703:ILE:HA	1:A:733:MET:O	2.15	0.47
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.49	0.47
1:B:543:LEU:HD21	1:B:627:TRP:CD1	2.44	0.47
1:B:545:ASP:C	1:B:545:ASP:OD1	2.57	0.47
1:B:594:ILE:HD11	1:B:602:GLU:H	1.79	0.47
1:B:651:ILE:HD11	1:B:759:ILE:HD13	1.96	0.47
1:A:543:LEU:HD12	1:A:567:LEU:HD13	1.97	0.47
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.45	0.47
1:A:115:LEU:HD11	1:A:155:VAL:HG11	1.97	0.47
1:A:506:ASN:N	1:A:506:ASN:HD22	2.12	0.47
1:A:712:HIS:O	1:A:713:PHE:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:C	1:B:97:GLU:N	2.70	0.47
1:B:479:LEU:HD22	1:B:480:TYR:N	2.30	0.47
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.98	0.47
1:A:58:TYR:CD1	1:A:60:LEU:HD12	2.50	0.47
1:A:513:LYS:HE2	1:A:515:ASP:HB2	1.97	0.47
1:B:235:LEU:HD23	1:B:255:PRO:N	2.30	0.47
1:A:98:PHE:HD2	1:A:100:HIS:O	1.97	0.46
1:B:305:TRP:CZ3	1:B:311:ILE:HG12	2.50	0.46
1:B:377:ASN:ND2	1:B:381:TYR:H	2.13	0.46
1:A:103:ASN:HB3	1:A:117:GLU:O	2.15	0.46
1:B:324:VAL:HG22	1:B:346:ILE:HG12	1.98	0.46
1:A:39:SER:HB2	1:A:508:GLN:HG3	1.95	0.46
1:A:219:ASN:HB2	3:A:915:HOH:O	2.14	0.46
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.98	0.46
1:B:49:LEU:HD12	1:B:49:LEU:HA	1.72	0.46
1:B:89:PHE:CE2	1:B:107:ILE:HD13	2.50	0.46
1:A:104:ASP:OD1	1:A:105:TYR:N	2.47	0.46
1:A:573:ILE:HD11	1:A:765:LEU:CD1	2.46	0.46
1:B:334:SER:C	1:B:336:ARG:H	2.24	0.46
1:B:444:CYS:HG	1:B:447:CYS:HG	0.53	0.46
1:A:377:ASN:HB3	1:A:396:PHE:CE1	2.51	0.46
1:A:592:HIS:HE1	3:A:929:HOH:O	1.98	0.45
1:B:420:ASN:C	1:B:420:ASN:ND2	2.74	0.45
1:A:612:GLN:O	1:A:615:LYS:HB2	2.17	0.45
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.98	0.45
1:B:269:PHE:CE1	1:B:286:GLN:HB2	2.52	0.45
1:B:429:ARG:NH1	1:B:456:TYR:OH	2.50	0.45
1:B:454:CYS:CB	1:B:472:CYS:HG	2.29	0.45
1:B:387:PHE:CD2	1:B:394:CYS:HB3	2.51	0.45
1:A:520:ASN:N	3:A:931:HOH:O	2.49	0.45
1:A:592:HIS:C	1:A:594:ILE:H	2.24	0.45
1:B:316:LEU:HD12	1:B:323:SER:HB3	1.99	0.45
1:A:202:VAL:HG22	1:A:257:PRO:HD2	1.98	0.45
1:B:405:ILE:HG12	1:B:429:ARG:NE	2.32	0.45
1:B:61:ARG:O	1:B:61:ARG:HG3	2.16	0.45
1:B:289:ALA:HB2	1:B:315:TRP:CH2	2.51	0.45
1:B:374:ILE:HD11	1:B:406:GLY:HA2	1.98	0.45
1:A:422:TYR:CD1	1:A:447:CYS:SG	3.10	0.45
1:A:434:ILE:N	1:A:434:ILE:CD1	2.79	0.45
1:A:588:ASP:HB3	1:A:592:HIS:CD2	2.52	0.45
1:B:680:LEU:C	1:B:680:LEU:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HG	1:A:49:LEU:HD22	1.99	0.45
1:A:321:ASN:O	1:A:348:MET:HA	2.17	0.45
1:B:614:SER:HA	1:B:619:VAL:CG2	2.46	0.45
1:A:158:SER:OG	1:A:163:LYS:HB2	2.17	0.44
1:A:463:LYS:O	1:A:464:GLU:HB2	2.17	0.44
1:A:72:GLN:HB2	1:A:77:LEU:HD22	1.99	0.44
1:A:40:ARG:HE	1:A:40:ARG:CA	2.29	0.44
1:A:60:LEU:HD11	1:A:469:GLN:CD	2.42	0.44
1:A:554:LYS:HE2	1:A:554:LYS:HB3	1.69	0.44
1:B:143:ILE:O	1:B:143:ILE:HG13	2.18	0.44
1:B:434:ILE:HD11	1:B:439:TYR:HD1	1.82	0.44
1:B:751:ILE:CG2	1:B:752:TYR:N	2.80	0.44
1:A:263:ASN:HD22	1:A:263:ASN:HA	1.61	0.44
1:B:479:LEU:HD22	1:B:479:LEU:C	2.43	0.44
1:A:60:LEU:HD11	1:A:469:GLN:NE2	2.32	0.44
1:A:134:ILE:HD11	1:A:148:ILE:HD11	2.00	0.44
1:B:256:TYR:CD1	1:B:256:TYR:C	2.96	0.44
1:B:471:ARG:HD3	1:B:480:TYR:HE2	1.82	0.44
1:B:519:LEU:O	1:B:520:ASN:C	2.61	0.44
1:A:109:PRO:HB2	1:A:160:VAL:HA	2.00	0.44
1:A:415:LEU:HD23	1:A:416:TYR:N	2.32	0.44
1:A:703:ILE:HG12	1:A:733:MET:HB3	1.99	0.44
1:B:63:ILE:HD11	1:B:69:LEU:CD1	2.47	0.44
1:B:142:LEU:HD12	1:B:142:LEU:N	2.33	0.44
1:B:170:ASN:O	1:B:196:ASN:HB2	2.18	0.44
1:A:177:GLU:HG3	1:A:180:LEU:HD22	1.99	0.43
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.88	0.43
1:B:680:LEU:O	1:B:683:TYR:HB2	2.18	0.43
1:A:49:LEU:HG	1:A:749:GLN:HG2	2.01	0.43
1:B:60:LEU:HD11	1:B:469:GLN:CD	2.42	0.43
1:B:184:ARG:HD3	1:B:187:TRP:CH2	2.52	0.43
1:B:651:ILE:CD1	1:B:759:ILE:HD13	2.48	0.43
1:A:377:ASN:HB3	1:A:396:PHE:CZ	2.53	0.43
1:B:208:PHE:HZ	1:B:300:LEU:HD12	1.83	0.43
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.18	0.43
1:A:185:ILE:HD12	1:A:271:VAL:HG11	2.00	0.43
1:A:434:ILE:CG2	1:A:442:VAL:HG22	2.42	0.43
1:A:513:LYS:O	1:A:527:GLN:HA	2.19	0.43
1:B:759:ILE:HG22	1:B:760:LYS:N	2.32	0.43
1:A:541:PRO:HB2	1:A:763:PHE:CE2	2.54	0.43
1:A:549:GLY:HA2	1:A:631:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ALA:HA	1:A:704:HIS:ND1	2.34	0.43
1:B:55:LEU:HD21	1:B:559:PHE:CE2	2.54	0.43
1:B:109:PRO:HG2	1:B:158:SER:O	2.18	0.43
1:B:680:LEU:HD13	1:B:684:ARG:HD2	2.01	0.43
1:A:105:TYR:HA	1:A:115:LEU:O	2.18	0.43
1:A:107:ILE:HG12	1:A:114:ILE:HD12	2.01	0.43
1:A:415:LEU:HD23	1:A:415:LEU:C	2.43	0.43
1:B:110:ASP:O	1:B:112:GLN:HG3	2.19	0.43
1:B:742:ILE:O	1:B:742:ILE:HG22	2.18	0.43
1:A:256:TYR:CD1	1:A:256:TYR:C	2.97	0.43
1:B:64:SER:HA	1:B:463:LYS:HD2	2.00	0.43
1:A:89:PHE:CE2	1:A:107:ILE:HD13	2.42	0.43
1:A:163:LYS:HZ2	1:A:273:THR:CG2	2.32	0.43
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.73	0.43
1:B:327:ILE:O	1:B:327:ILE:HG22	2.19	0.43
1:B:459:VAL:CG2	1:B:460:SER:N	2.81	0.43
1:A:567:LEU:CD2	1:A:573:ILE:HD12	2.42	0.42
1:B:137:LEU:O	1:B:139:LYS:N	2.52	0.42
1:B:306:ALA:CB	1:B:310:ARG:HG2	2.47	0.42
1:B:397:ILE:HG23	1:B:439:TYR:CD1	2.54	0.42
1:A:508:GLN:NE2	1:A:533:HIS:CE1	2.81	0.42
1:A:522:THR:HB	1:A:524:PHE:CE2	2.55	0.42
1:B:325:MET:HE2	1:B:327:ILE:CD1	2.47	0.42
1:B:471:ARG:HD3	1:B:480:TYR:CE2	2.54	0.42
1:A:113:PHE:HE2	1:A:162:HIS:ND1	2.17	0.42
1:A:417:TYR:HE1	1:A:434:ILE:HG23	1.84	0.42
1:A:504:LEU:HD22	1:A:509:MET:SD	2.60	0.42
1:B:446:SER:HA	1:B:449:LEU:CD1	2.49	0.42
1:B:102:ILE:HD13	1:B:116:LEU:HD22	2.01	0.42
1:A:382:ARG:HH11	1:A:382:ARG:HG2	1.84	0.42
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.54	0.42
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.88	0.42
1:B:289:ALA:HB2	1:B:315:TRP:CZ3	2.55	0.42
1:B:715:GLN:HE21	1:B:715:GLN:HB3	1.66	0.42
1:B:276:LEU:HD23	1:B:282:ALA:HB2	2.02	0.42
1:A:62:TRP:CG	1:A:462:SER:HA	2.55	0.42
1:B:236:ILE:HD13	1:B:238:TYR:HD1	1.85	0.42
1:B:429:ARG:NH2	3:B:911:HOH:O	2.53	0.42
1:B:55:LEU:HD21	1:B:559:PHE:HE2	1.85	0.42
1:B:71:LYS:HD3	1:B:105:TYR:HE2	1.84	0.42
1:B:602:GLU:O	1:B:606:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HA	1:A:252:VAL:O	2.20	0.42
1:A:401:THR:O	1:A:401:THR:HG22	2.18	0.42
1:B:522:THR:HG22	1:B:523:LYS:N	2.34	0.42
1:A:39:SER:HB3	1:A:506:ASN:O	2.20	0.41
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.19	0.41
1:B:608:GLU:O	1:B:612:GLN:HG2	2.20	0.41
1:B:614:SER:HA	1:B:619:VAL:HG22	2.01	0.41
1:A:82:GLU:HB2	1:A:467:TYR:OH	2.21	0.41
1:A:528:MET:HG2	1:A:574:ILE:CG2	2.50	0.41
1:A:573:ILE:HD11	1:A:765:LEU:HD11	2.02	0.41
1:B:418:ILE:HA	1:B:430:ASN:O	2.21	0.41
1:B:461:PHE:CE1	1:B:468:TYR:HB3	2.55	0.41
1:B:626:ILE:O	1:B:650:GLY:HA2	2.20	0.41
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.55	0.41
1:B:425:MET:CE	1:B:514:LEU:HD13	2.50	0.41
1:B:543:LEU:HD12	1:B:567:LEU:HD13	2.02	0.41
1:B:758:PHE:O	1:B:761:GLN:HG3	2.20	0.41
1:A:614:SER:O	1:A:615:LYS:C	2.61	0.41
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.77	0.41
1:A:594:ILE:O	1:A:594:ILE:HG23	2.20	0.41
1:B:358:ARG:NH2	3:B:912:HOH:O	2.53	0.41
1:B:515:ASP:HB3	1:B:526:TYR:CZ	2.56	0.41
1:B:263:ASN:HD22	1:B:263:ASN:HA	1.63	0.41
1:B:304:THR:HB	1:B:312:SER:OG	2.20	0.41
1:B:383:HIS:HE1	1:B:400:GLY:O	2.04	0.41
1:A:118:TYR:O	1:A:119:ASN:HB2	2.21	0.41
1:A:150:ASN:O	1:A:151:ASN:HB2	2.19	0.41
1:A:219:ASN:ND2	3:A:908:HOH:O	2.54	0.41
1:B:58:TYR:CD1	1:B:60:LEU:HD12	2.55	0.41
1:A:150:ASN:ND2	3:A:919:HOH:O	2.46	0.41
1:A:197:GLY:C	1:A:213:ALA:HB3	2.46	0.41
1:A:253:ARG:NH2	1:B:253:ARG:NH1	2.59	0.41
1:A:310:ARG:HG3	1:A:329:ASP:OD1	2.21	0.41
1:A:449:LEU:HD23	1:A:449:LEU:HA	1.75	0.41
1:B:118:TYR:O	1:B:119:ASN:HB2	2.21	0.41
1:B:454:CYS:HB3	1:B:472:CYS:HB2	2.03	0.41
1:B:598:LEU:O	1:B:682:HIS:HE1	2.04	0.41
1:A:253:ARG:NH1	1:B:253:ARG:HH12	2.19	0.41
1:B:110:ASP:O	1:B:112:GLN:N	2.48	0.41
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.39	0.40
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:ILE:O	1:A:650:GLY:CA	2.69	0.40
1:B:393:ASP:HB3	1:B:394:CYS:H	1.74	0.40
1:B:674:PRO:O	1:B:680:LEU:HD23	2.21	0.40
1:A:39:SER:O	1:A:40:ARG:HB2	2.21	0.40
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.51	0.40
1:B:429:ARG:CZ	3:B:911:HOH:O	2.69	0.40
1:A:200:ASP:OD1	1:A:200:ASP:C	2.65	0.40
1:A:654:ALA:HA	1:A:704:HIS:CE1	2.57	0.40
1:A:728:VAL:O	1:B:750:HIS:HE1	2.03	0.40
1:B:248:TYR:HA	1:B:249:PRO:HD3	1.99	0.40
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.85	0.40
1:A:322:TYR:HD2	1:A:348:MET:HG2	1.86	0.40
1:A:435:GLN:HE22	1:A:441:LYS:HD3	1.85	0.40
1:A:674:PRO:O	1:A:680:LEU:HB2	2.21	0.40
1:B:276:LEU:CD2	1:B:282:ALA:HB2	2.50	0.40
1:B:158:SER:HA	1:B:216:TRP:CD1	2.57	0.40
1:B:626:ILE:O	1:B:650:GLY:CA	2.70	0.40
1:B:630:SER:OG	1:B:631:TYR:N	2.55	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	726/728 (100%)	672 (93%)	51 (7%)	3 (0%)	30	34
1	B	726/728 (100%)	687 (95%)	37 (5%)	2 (0%)	36	43
All	All	1452/1456 (100%)	1359 (94%)	88 (6%)	5 (0%)	36	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	521	GLU
1	A	742	ILE
1	B	138	ASN
1	B	140	ARG
1	A	438	ASP

5.3.2 Protein sidechains ⓘ

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	653/653 (100%)	605 (93%)	48 (7%)	13	14
1	B	653/653 (100%)	607 (93%)	46 (7%)	14	15
All	All	1306/1306 (100%)	1212 (93%)	94 (7%)	13	14

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	51	ASN
1	A	57	LEU
1	A	60	LEU
1	A	63	ILE
1	A	72	GLN
1	A	75	ASN
1	A	108	SER
1	A	115	LEU
1	A	140	ARG
1	A	142	LEU
1	A	180	LEU
1	A	190	LYS
1	A	202	VAL
1	A	223	LEU
1	A	246	LEU
1	A	263	ASN
1	A	294	LEU
1	A	300	LEU

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Mol	Chain	Res	Type
1	A	316	LEU
1	A	326	ASP
1	A	332	GLU
1	A	340	LEU
1	A	377	ASN
1	A	382	ARG
1	A	385	CYS
1	A	410	LEU
1	A	420	ASN
1	A	431	LEU
1	A	434	ILE
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	484	SER
1	A	500	LEU
1	A	502	LYS
1	A	513	LYS
1	A	528	MET
1	A	543	LEU
1	A	544	LEU
1	A	589	LYS
1	A	594	ILE
1	A	597	ARG
1	A	621	ASN
1	A	677	GLU
1	A	696	LYS
1	A	715	GLN
1	A	736	THR
1	B	40	ARG
1	B	41	LYS
1	B	42	THR
1	B	49	LEU
1	B	57	LEU
1	B	60	LEU
1	B	78	VAL
1	B	91	GLU
1	B	144	THR
1	B	214	LEU
1	B	223	LEU
1	B	231	THR
1	B	236	ILE

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Mol	Chain	Res	Type
1	B	246	LEU
1	B	263	ASN
1	B	311	ILE
1	B	326	ASP
1	B	327	ILE
1	B	336	ARG
1	B	376	SER
1	B	377	ASN
1	B	378	GLU
1	B	385	CYS
1	B	389	ILE
1	B	391	LYS
1	B	420	ASN
1	B	434	ILE
1	B	443	THR
1	B	472	CYS
1	B	479	LEU
1	B	500	LEU
1	B	514	LEU
1	B	519	LEU
1	B	542	LEU
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	577	SER
1	B	594	ILE
1	B	619	VAL
1	B	679	ASN
1	B	680	LEU
1	B	684	ARG
1	B	715	GLN
1	B	759	ILE
1	B	762	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	141	GLN
1	A	263	ASN
1	A	298	HIS
1	A	314	GLN

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Mol	Chain	Res	Type
1	A	363	HIS
1	A	377	ASN
1	A	388	GLN
1	A	420	ASN
1	A	435	GLN
1	A	469	GLN
1	A	483	HIS
1	A	506	ASN
1	A	508	GLN
1	A	533	HIS
1	A	586	GLN
1	A	592	HIS
1	A	612	GLN
1	A	679	ASN
1	A	715	GLN
1	A	731	GLN
1	A	749	GLN
1	A	750	HIS
1	A	757	HIS
1	B	72	GLN
1	B	75	ASN
1	B	103	ASN
1	B	169	ASN
1	B	263	ASN
1	B	298	HIS
1	B	345	HIS
1	B	363	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	435	GLN
1	B	483	HIS
1	B	562	ASN
1	B	586	GLN
1	B	595	ASN
1	B	612	GLN
1	B	679	ASN
1	B	682	HIS
1	B	715	GLN
1	B	731	GLN
1	B	750	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	1MD	B	801	-	27,29,29	2.01	9 (33%)	37,43,43	2.52	16 (43%)
2	1MD	A	801	-	27,29,29	1.97	9 (33%)	37,43,43	2.20	10 (27%)

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	1MD	B	801	-	-	1/13/26/26	0/3/3/3
2	1MD	A	801	-	-	0/13/26/26	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	1MD	C18-C17	4.88	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	1MD	C20-C19	4.40	1.45	1.38
2	A	801	1MD	C18-C17	3.90	1.45	1.38
2	B	801	1MD	C19-CL2	-3.38	1.66	1.74
2	A	801	1MD	C18-C19	3.17	1.43	1.38
2	B	801	1MD	C7-N2	2.99	1.38	1.34
2	B	801	1MD	C20-C21	2.95	1.43	1.38
2	A	801	1MD	C7-N2	2.92	1.38	1.34
2	A	801	1MD	C20-C21	2.88	1.43	1.38
2	A	801	1MD	C2-C3	2.74	1.44	1.39
2	B	801	1MD	C14-C21	2.74	1.44	1.39
2	B	801	1MD	C18-C19	2.72	1.43	1.38
2	B	801	1MD	C3-N4	2.65	1.38	1.34
2	A	801	1MD	C14-C21	2.63	1.44	1.39
2	B	801	1MD	C2-C3	2.63	1.43	1.39
2	B	801	1MD	C17-C14	2.57	1.43	1.40
2	A	801	1MD	C17-C14	2.41	1.43	1.40
2	A	801	1MD	C1-C2	2.02	1.44	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	1MD	C10-N1-C9	-6.88	117.14	123.76
2	B	801	1MD	C10-N1-C9	-5.90	118.08	123.76
2	B	801	1MD	C20-C21-C14	5.43	126.19	121.97
2	A	801	1MD	C20-C21-C14	5.10	125.93	121.97
2	A	801	1MD	C21-C20-C19	-4.60	113.53	118.72
2	B	801	1MD	C21-C20-C19	-4.27	113.90	118.72
2	B	801	1MD	C20-C21-CL1	-4.23	111.52	118.45
2	B	801	1MD	C13-C3-C2	-4.15	116.80	122.31
2	B	801	1MD	C5-N1-C10	4.01	128.34	122.64
2	B	801	1MD	C7-C10-N1	3.93	116.70	111.55
2	B	801	1MD	C20-C19-CL2	-3.49	114.79	119.17
2	B	801	1MD	C3-N4-C6	-3.49	114.22	118.66
2	A	801	1MD	C10-C7-N2	-3.00	113.32	116.69
2	B	801	1MD	C15-C2-C3	-2.99	116.10	119.69
2	A	801	1MD	C13-C3-N4	-2.68	112.37	116.53
2	A	801	1MD	C20-C21-CL1	-2.68	114.07	118.45
2	A	801	1MD	O2-C7-N2	2.58	125.99	121.89
2	A	801	1MD	C5-N1-C10	2.58	126.30	122.64
2	B	801	1MD	C4-C1-C2	-2.51	114.84	117.99
2	A	801	1MD	C7-C10-N1	-2.29	108.54	111.55
2	B	801	1MD	C5-C6-C4	-2.21	107.94	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	1MD	C18-C19-C20	2.19	124.40	121.53
2	A	801	1MD	C8-N2-C7	-2.18	115.37	121.73
2	B	801	1MD	C1-C14-C21	-2.06	119.94	122.31
2	B	801	1MD	C14-C1-C2	2.04	123.83	120.61
2	B	801	1MD	C10-C7-N2	-2.01	114.43	116.69

There are no chirality outliers.

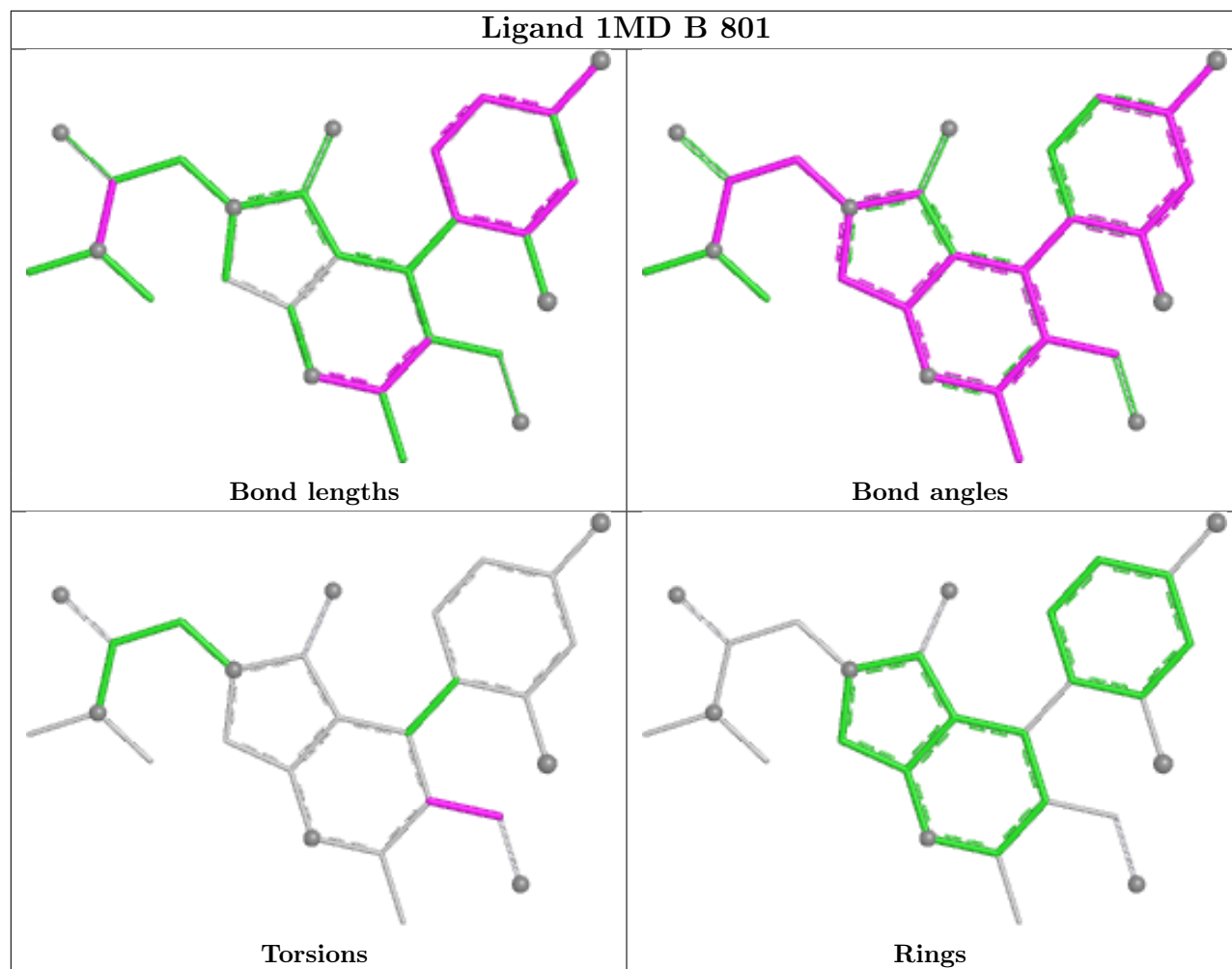
All (1) torsion outliers are listed below:

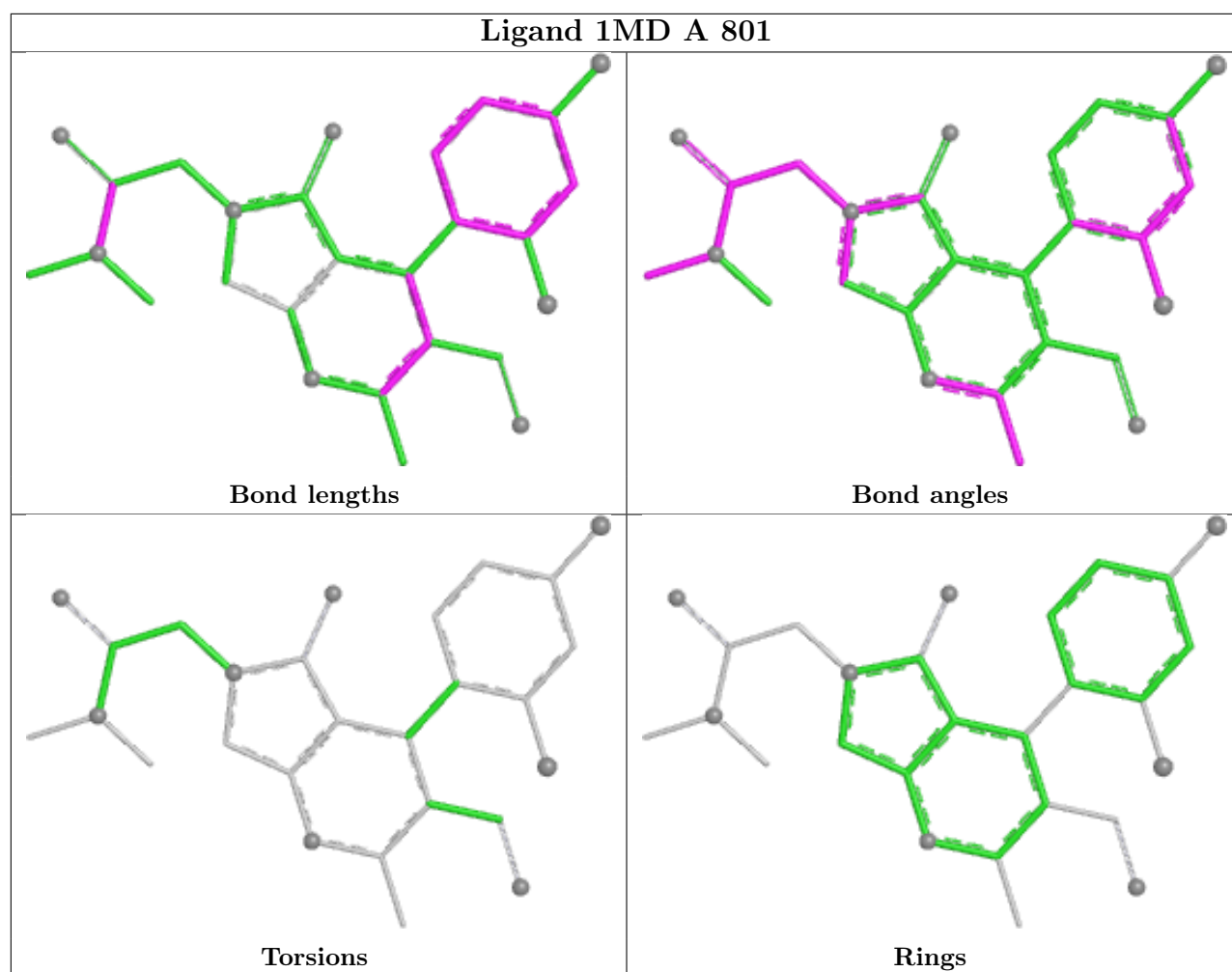
Mol	Chain	Res	Type	Atoms
2	B	801	1MD	N16-C15-C2-C1

There are no ring outliers.

No monomer is involved in short contacts.

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 than 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.





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, 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	728/728 (100%)	0.26	45 (6%)	26 30	20, 36, 80, 152	0
1	B	728/728 (100%)	0.60	57 (7%)	19 21	21, 41, 81, 144	0
All	All	1456/1456 (100%)	0.43	102 (7%)	22 25	20, 39, 81, 152	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	766	PRO	6.8
1	A	142	LEU	6.0
1	B	279	VAL	5.0
1	A	489	LYS	4.9
1	B	143	ILE	4.9
1	A	39	SER	4.4
1	B	145	GLU	4.3
1	B	61	ARG	4.3
1	A	350	THR	4.2
1	B	766	PRO	3.9
1	A	40	ARG	3.9
1	B	110	ASP	3.8
1	A	521	GLU	3.7
1	A	677	GLU	3.7
1	B	141	GLN	3.7
1	B	696	LYS	3.7
1	A	765	LEU	3.6
1	B	273	THR	3.5
1	A	91	GLU	3.5
1	B	144	THR	3.4
1	B	597	ARG	3.2
1	B	340	LEU	3.2
1	B	138	ASN	3.2
1	B	39	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	145	GLU	3.1
1	B	521	GLU	3.1
1	B	321	ASN	3.1
1	B	350	THR	3.1
1	A	138	ASN	3.1
1	B	379	GLU	3.0
1	B	66	HIS	3.0
1	B	142	LEU	3.0
1	B	140	ARG	3.0
1	A	73	GLU	3.0
1	B	91	GLU	3.0
1	B	393	ASP	3.0
1	A	140	ARG	2.9
1	B	765	LEU	2.9
1	A	141	GLN	2.9
1	A	160	VAL	2.9
1	A	536	LYS	2.9
1	B	392	LYS	2.8
1	B	536	LYS	2.8
1	B	330	TYR	2.8
1	A	243	ASP	2.8
1	B	617	GLY	2.8
1	B	520	ASN	2.7
1	B	97	GLU	2.7
1	B	389	ILE	2.6
1	B	53	TYR	2.6
1	B	63	ILE	2.5
1	B	280	THR	2.5
1	A	96	ASP	2.5
1	B	278	SER	2.5
1	A	519	LEU	2.5
1	B	92	ASN	2.4
1	A	471	ARG	2.4
1	A	392	LYS	2.4
1	B	764	SER	2.4
1	A	520	ASN	2.4
1	A	280	THR	2.4
1	A	271	VAL	2.4
1	B	613	PHE	2.4
1	A	62	TRP	2.4
1	A	281	ASN	2.3
1	B	219	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	99	GLY	2.3
1	A	57	LEU	2.3
1	A	502	LYS	2.3
1	B	441	LYS	2.3
1	A	54	ARG	2.3
1	A	105	TYR	2.3
1	A	464	GLU	2.2
1	B	135	TYR	2.2
1	B	489	LYS	2.2
1	B	397	ILE	2.2
1	A	764	SER	2.2
1	A	219	ASN	2.2
1	A	332	GLU	2.2
1	A	615	LYS	2.2
1	B	761	GLN	2.2
1	A	278	SER	2.2
1	A	342	ALA	2.2
1	B	42	THR	2.2
1	B	277	SER	2.2
1	B	338	ASN	2.1
1	B	332	GLU	2.1
1	A	144	THR	2.1
1	A	348	MET	2.1
1	A	487	ASN	2.1
1	B	614	SER	2.1
1	B	111	GLY	2.1
1	B	336	ARG	2.1
1	A	334	SER	2.0
1	B	59	SER	2.0
1	A	378	GLU	2.0
1	A	114	ILE	2.0
1	B	41	LYS	2.0
1	B	615	LYS	2.0
1	B	182	SER	2.0
1	B	90	LEU	2.0
1	B	685	ASN	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

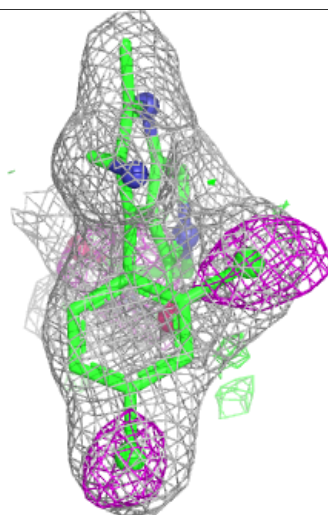
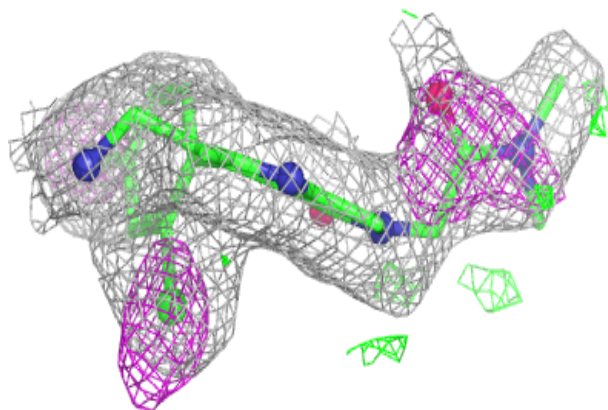
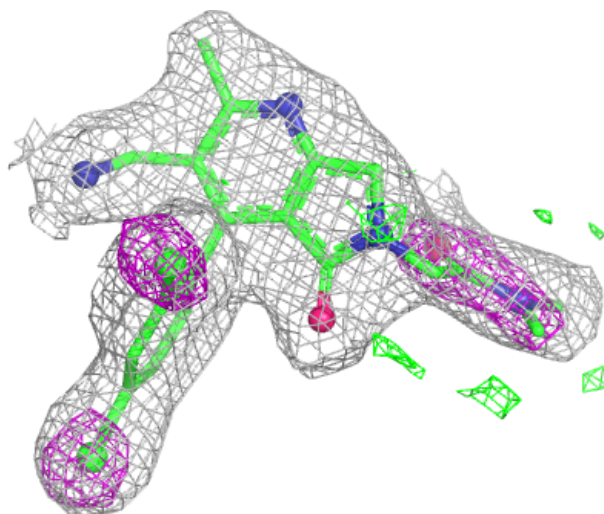
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	1MD	A	801	27/27	0.93	0.10	21,21,21,21	0
2	1MD	B	801	27/27	0.94	0.09	21,21,21,21	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.

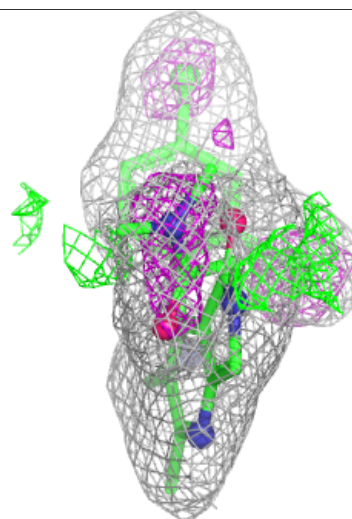
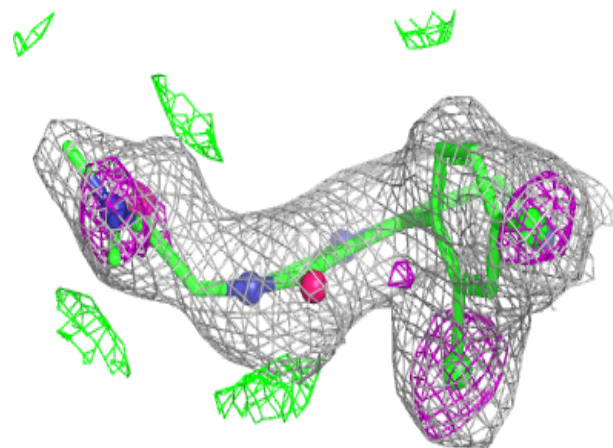
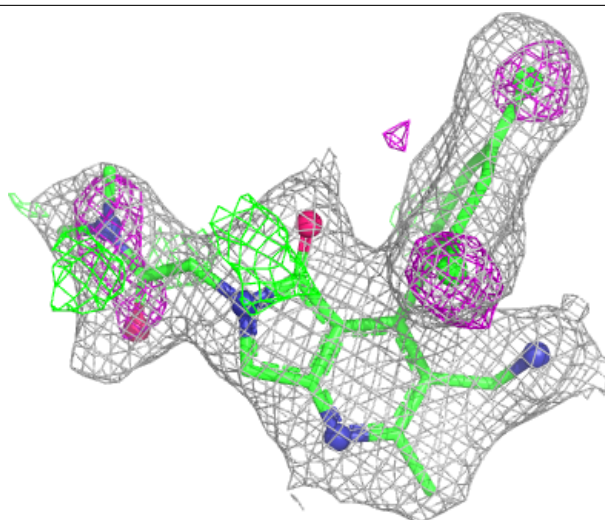
Electron density around 1MD A 801:

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



Electron density around 1MD B 801:

$2mF_o-DF_c$ (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.