



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 PM UTC

PDB ID : 7FVS / pdb_00007fvs
Title : Crystal Structure of S. aureus gyrase in complex with 4-[[1-[(1-chloro-6,7-dihydro-5H-cyclopenta[c]pyridin-6-yl)methyl]azetidin-3-yl]methylamino]-6-fluorochromen-2-one
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Deposited on : 2023-04-18
Resolution : 2.16 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 ⓘ](#)) 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

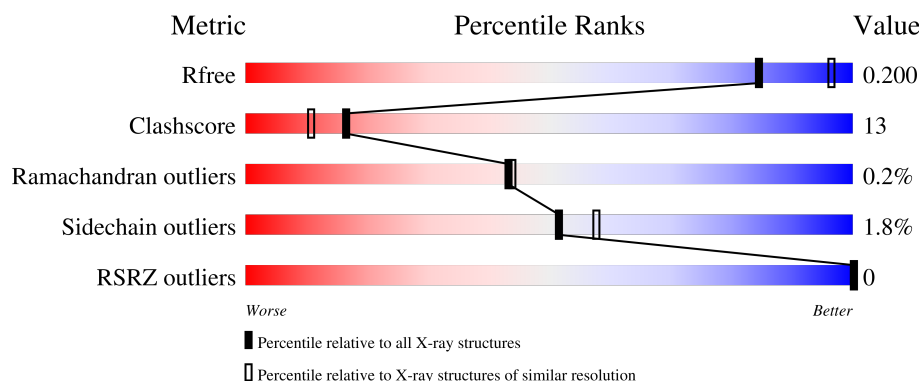
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	692	 71% 26% . .
1	B	692	 67% 29% . .
2	C	20	 70% 30%
2	D	20	 55% 45%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	B	1503	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11927 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 DNA gyrase subunit B,DNA gyrase subunit A Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	0	0
			5313	3314	957	1017	25			
1	B	671	Total	C	N	O	S	0	0	0
			5318	3316	958	1019	25			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	MET	-	initiating methionine	UNP P66937
A	?	-	LEU	deletion	UNP P66937
A	?	-	TYR	deletion	UNP P66937
A	?	-	LYS	deletion	UNP P66937
A	?	-	LEU	deletion	UNP P66937
A	?	-	THR	deletion	UNP P66937
A	?	-	GLN	deletion	UNP P66937
A	?	-	GLY	deletion	UNP P66937
A	?	-	LYS	deletion	UNP P66937
A	?	-	GLN	deletion	UNP P66937
A	?	-	LYS	deletion	UNP P66937
A	?	-	TYR	deletion	UNP P66937
A	?	-	TYR	deletion	UNP P66937
A	?	-	VAL	deletion	UNP P66937
A	?	-	TYR	deletion	UNP P66937
A	?	-	ASN	deletion	UNP P66937
A	?	-	ASP	deletion	UNP P66937
A	?	-	ARG	deletion	UNP P66937
A	?	-	GLU	deletion	UNP P66937
A	?	-	LEU	deletion	UNP P66937
A	?	-	ASP	deletion	UNP P66937
A	?	-	LYS	deletion	UNP P66937
A	?	-	LEU	deletion	UNP P66937
A	?	-	LYS	deletion	UNP P66937
A	?	-	SER	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P66937
A	?	-	LEU	deletion	UNP P66937
A	?	-	ASN	deletion	UNP P66937
A	?	-	PRO	deletion	UNP P66937
A	?	-	THR	deletion	UNP P66937
A	?	-	PRO	deletion	UNP P66937
A	?	-	LYS	deletion	UNP P66937
A	?	-	TRP	deletion	UNP P66937
A	?	-	SER	deletion	UNP P66937
A	?	-	ILE	deletion	UNP P66937
A	544	THR	ALA	conflict	UNP P66937
A	545	GLY	ARG	conflict	UNP P66937
A	1123	PHE	TYR	engineered mutation	UNP Q99XG5
B	409	MET	-	initiating methionine	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	THR	deletion	UNP P66937
B	?	-	GLN	deletion	UNP P66937
B	?	-	GLY	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	GLN	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	VAL	deletion	UNP P66937
B	?	-	TYR	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	ARG	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASP	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937
B	?	-	GLU	deletion	UNP P66937
B	?	-	LEU	deletion	UNP P66937
B	?	-	ASN	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP P66937
B	?	-	PRO	deletion	UNP P66937
B	?	-	LYS	deletion	UNP P66937
B	?	-	TRP	deletion	UNP P66937
B	?	-	SER	deletion	UNP P66937
B	?	-	ILE	deletion	UNP P66937
B	544	THR	ALA	conflict	UNP P66937
B	545	GLY	ARG	conflict	UNP P66937
B	1123	PHE	TYR	engineered mutation	UNP Q99XG5

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			407	193	77	118	19			
2	D	20	Total	C	N	O	P	0	0	0
			390	183	75	113	19			

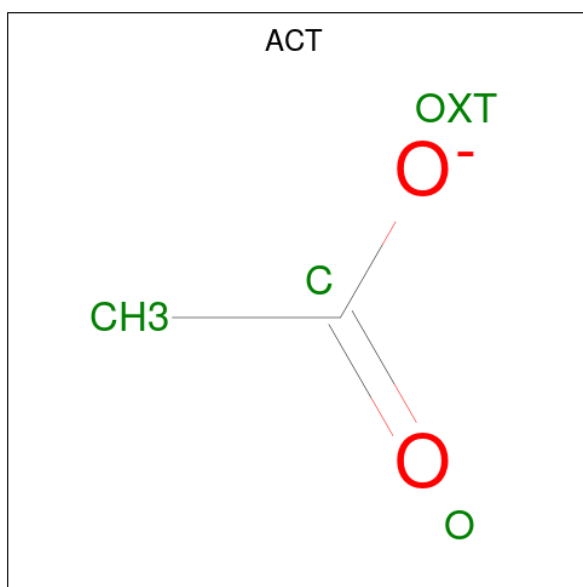
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	2	Total	Mn	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

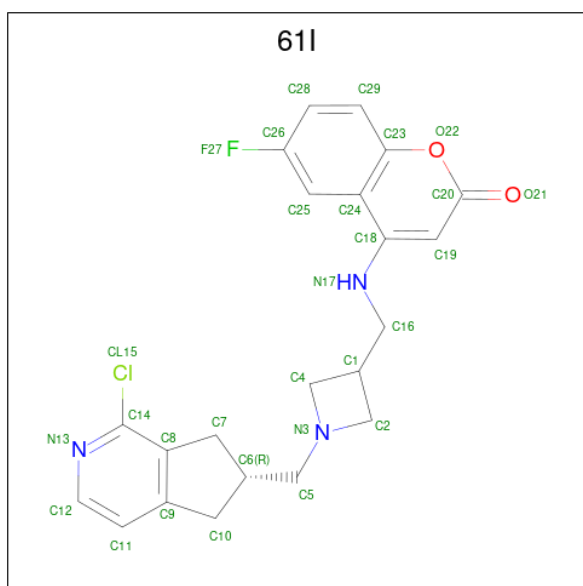
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 4-[[[(1-[(6R)-1-chloro-6,7-dihydro-5H-cyclopenta[c]pyridin-6-yl)methyl]azetidin-3-yl)methyl]amino]-6-fluoro-2H-1-benzopyran-2-one (CCD ID: 61I) (formula: C₂₂H₂₁ClFN₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total	C	Cl	F	N	O	0	0
			29	22	1	1	3	2		

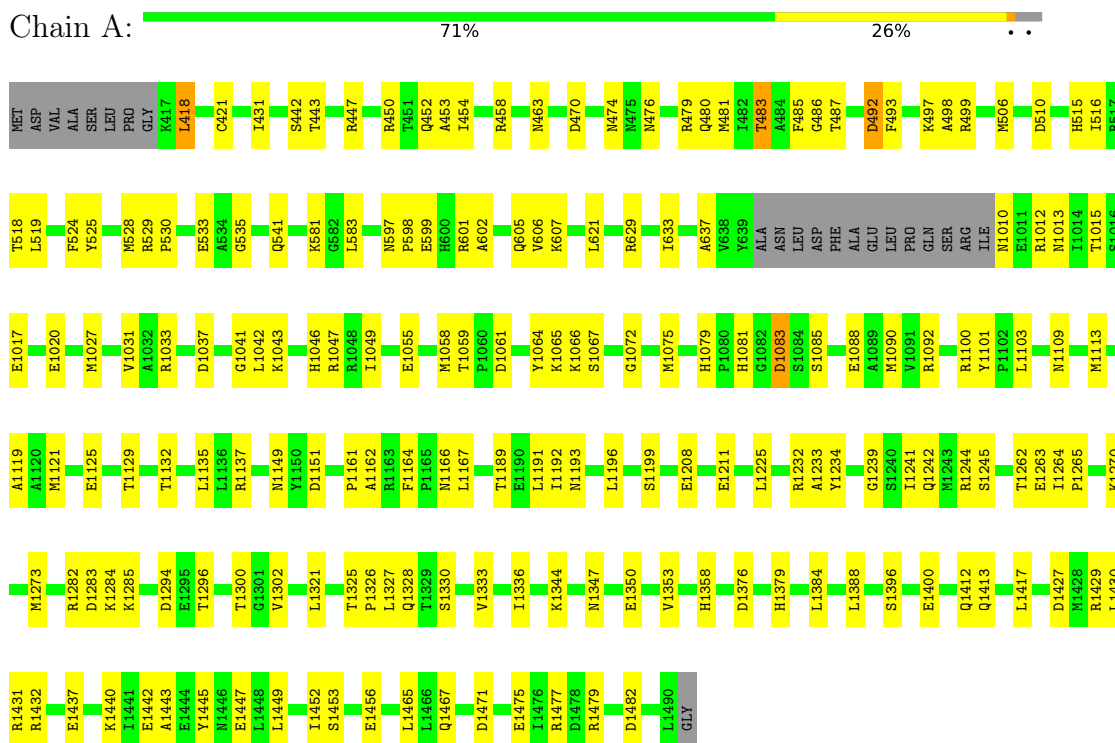
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	205	Total 205	O 205	0	0
7	B	197	Total 197	O 197	0	0
7	C	30	Total 30	O 30	0	0
7	D	30	Total 30	O 30	0	0

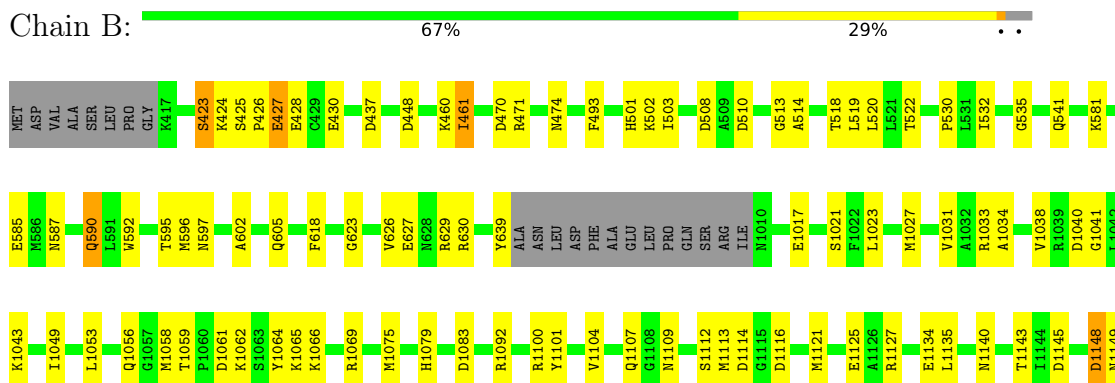
3 Residue-property plots

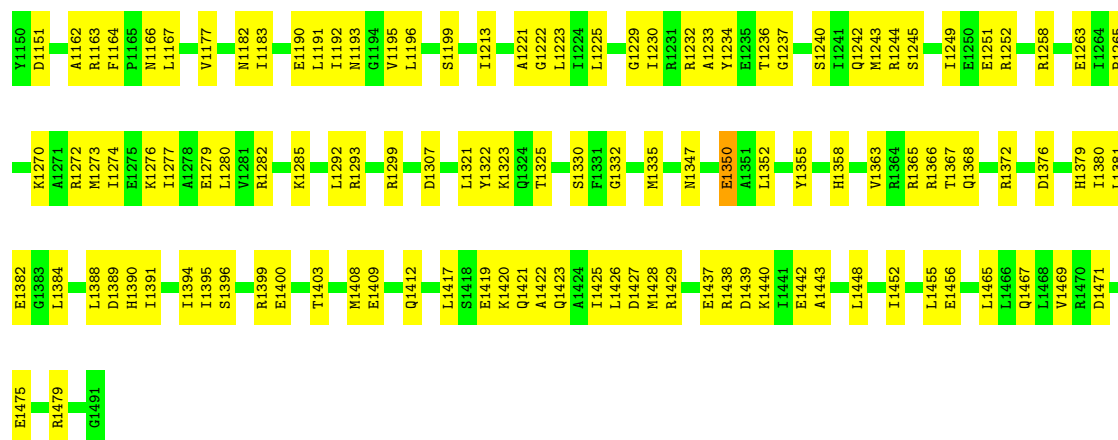
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



- Molecule 1: DNA gyrase subunit B,DNA gyrase subunit A Chimera





- Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')



- Molecule 2: DNA (5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*GP*CP*CP*CP*TP*AP*CP*GP*GP*CP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	92.92Å 92.92Å 407.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.47 – 2.16 80.47 – 2.16	Depositor EDS
% Data completeness (in resolution range)	95.6 (80.47-2.16) 94.6 (80.47-2.16)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.89 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.12rc1 _2801	Depositor
R, R_{free}	0.185 , 0.221 0.175 , 0.200	Depositor DCC
R_{free} test set	5099 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.356 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.330 for k,h,-l	Depositor
Outliers	0 of 101251 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11927	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, CL, 6II, ACT

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	0.47	0/5385	0.59	0/7254
1	B	0.48	0/5390	0.59	1/7259 (0.0%)
2	C	0.47	0/456	0.60	0/702
2	D	0.61	0/437	0.64	0/672
All	All	0.48	0/11668	0.59	1/15887 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1221	ALA	CB-CA-C	-6.97	107.74	117.23

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	5313	0	5366	128	0
1	B	5318	0	5369	155	0
2	C	407	0	225	7	0
2	D	390	0	212	14	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	1	0
5	B	4	0	3	2	0
6	B	29	0	0	0	0
7	A	205	0	0	20	2
7	B	197	0	0	21	2
7	C	30	0	0	2	0
7	D	30	0	0	2	0
All	All	11927	0	11175	287	2

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 13.

All (287) 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:447:ARG:NH2	1:A:452:GLN:O	2.11	0.83
1:A:535:GLY:O	1:A:605:GLN:NE2	2.10	0.82
1:B:470:ASP:O	1:B:474:ASN:ND2	2.13	0.81
1:B:1323:LYS:O	7:B:1601:HOH:O	1.99	0.79
1:B:1439:ASP:O	1:B:1443:ALA:N	2.14	0.79
1:B:1350:GLU:OE1	7:B:1603:HOH:O	2.00	0.78
4:A:1502:CL:CL	7:B:1702:HOH:O	2.40	0.75
2:C:17:DG:N3	7:C:101:HOH:O	2.20	0.75
1:A:1055:GLU:OE2	7:A:1601:HOH:O	2.05	0.73
1:B:1321:LEU:O	1:B:1325:THR:OG1	2.03	0.73
1:B:430:GLU:HG2	1:B:502:LYS:HB2	1.69	0.73
1:A:1475:GLU:OE1	1:A:1479:ARG:NH2	2.22	0.73
1:B:1083:ASP:HB2	1:B:1121:MET:HE1	1.72	0.72
1:A:1413:GLN:O	7:A:1602:HOH:O	2.09	0.70
1:A:1429:ARG:NH1	1:B:1427:ASP:O	2.25	0.70
1:A:1273:MET:HG3	1:A:1326:PRO:HD2	1.74	0.69
1:B:1062:LYS:O	1:B:1127:ARG:NH1	2.22	0.69
1:B:461:ILE:HG22	1:B:519:LEU:HB3	1.74	0.68
1:A:541:GLN:NE2	1:A:602:ALA:O	2.25	0.68
1:A:1242:GLN:OE1	1:A:1328:GLN:NE2	2.24	0.68
1:B:541:GLN:NE2	1:B:602:ALA:O	2.24	0.67
1:A:1193:ASN:OD1	1:A:1477:ARG:NH1	2.28	0.66
1:B:448:ASP:OD2	7:B:1604:HOH:O	2.12	0.66
1:B:1064:TYR:HB3	1:B:1125:GLU:HB3	1.78	0.66
1:B:1467:GLN:NE2	1:B:1471:ASP:OD1	2.28	0.65
1:B:1140:ASN:O	7:B:1605:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:LEU:HB3	1:A:1327:LEU:HD12	1.79	0.65
1:B:1376:ASP:O	7:B:1607:HOH:O	2.14	0.65
1:A:1135:LEU:HD23	1:A:1162:ALA:HA	1.78	0.65
1:A:1270:LYS:NZ	1:A:1294:ASP:OD2	2.30	0.64
1:A:1075:MET:O	7:A:1603:HOH:O	2.14	0.64
1:B:471:ARG:NH2	2:D:14:DT:OP1	2.28	0.64
1:B:1183:ILE:HG12	1:B:1335:MET:HG2	1.79	0.64
1:B:1104:VAL:O	7:B:1606:HOH:O	2.14	0.64
2:D:7:DA:N6	7:D:102:HOH:O	2.23	0.64
1:B:1234:TYR:O	1:B:1347:ASN:HB2	1.98	0.63
1:A:1344:LYS:NZ	1:A:1350:GLU:OE2	2.32	0.63
1:B:427:GLU:OE1	1:B:428:GLU:N	2.31	0.63
1:A:1233:ALA:HB1	1:A:1333:VAL:HG11	1.79	0.62
1:A:1353:VAL:O	7:A:1605:HOH:O	2.16	0.62
1:A:1432:ARG:NH1	7:A:1604:HOH:O	2.15	0.62
1:B:1475:GLU:CD	1:B:1479:ARG:HH21	2.06	0.62
1:B:1389:ASP:CG	1:B:1438:ARG:HH21	2.08	0.62
1:B:1059:THR:OG1	1:B:1061:ASP:OD1	2.16	0.62
1:A:492:ASP:OD1	1:A:492:ASP:N	2.29	0.61
1:A:1046:HIS:ND1	7:A:1627:HOH:O	2.31	0.61
1:A:516:ILE:HA	1:A:519:LEU:HD12	1.82	0.61
1:B:1196:LEU:O	1:B:1199:SER:OG	2.18	0.60
1:B:1038:VAL:HA	1:B:1167:LEU:HD22	1.84	0.60
1:A:1109:ASN:HB3	1:A:1119:ALA:HB2	1.83	0.60
1:A:1467:GLN:NE2	1:A:1471:ASP:OD1	2.34	0.60
1:B:1017:GLU:OE2	1:B:1021:SER:OG	2.18	0.59
1:A:1482:ASP:OD2	7:A:1606:HOH:O	2.17	0.58
1:B:1379:HIS:O	1:B:1421:GLN:NE2	2.33	0.58
1:B:1092:ARG:NH2	7:B:1627:HOH:O	2.33	0.58
1:A:1208:GLU:HA	1:A:1211:GLU:OE1	2.03	0.57
1:A:1100:ARG:HG3	1:A:1101:TYR:CE2	2.38	0.57
1:B:1145:ASP:OD1	1:B:1365:ARG:NH1	2.31	0.57
1:B:1380:ILE:HD11	1:B:1420:LYS:HB3	1.86	0.57
1:A:479:ARG:O	1:A:483:THR:OG1	2.19	0.57
1:A:1232:ARG:CZ	1:A:1239:GLY:HA2	2.34	0.57
1:B:1439:ASP:HA	1:B:1442:GLU:HB3	1.87	0.56
1:A:1103:LEU:O	1:A:1132:THR:OG1	2.18	0.56
1:A:1137:ARG:HD3	7:A:1661:HOH:O	2.06	0.56
1:A:1012:ARG:NH2	1:A:1020:GLU:OE2	2.31	0.56
1:B:427:GLU:HA	1:B:501:HIS:CG	2.40	0.56
1:B:510:ASP:OD1	1:B:513:GLY:N	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ASN:OD1	1:A:599:GLU:HG3	2.06	0.55
1:A:1196:LEU:O	1:A:1199:SER:OG	2.24	0.55
1:B:1135:LEU:HD23	1:B:1162:ALA:HA	1.88	0.55
1:A:1059:THR:OG1	1:A:1061:ASP:OD1	2.18	0.55
1:B:1395:ILE:O	1:B:1399:ARG:HG3	2.06	0.55
1:A:458:ARG:NE	2:D:10:DG:H4'	2.21	0.55
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.40	0.54
1:B:1100:ARG:HG3	1:B:1101:TYR:CE2	2.42	0.54
1:A:1135:LEU:HG	1:A:1164:PHE:CE2	2.43	0.53
1:A:1149:ASN:ND2	1:A:1151:ASP:OD1	2.42	0.53
1:B:626:VAL:HG11	2:D:17:DG:H3'	1.88	0.53
1:B:522:THR:HA	1:B:618:PHE:CE1	2.44	0.53
1:B:1140:ASN:N	5:B:1503:ACT:O	2.39	0.53
1:B:1272:ARG:HG2	1:B:1276:LYS:HE3	1.91	0.53
1:A:515:HIS:O	1:A:518:THR:OG1	2.27	0.53
1:A:1242:GLN:NE2	7:A:1624:HOH:O	2.30	0.52
1:B:460:LYS:NZ	7:B:1617:HOH:O	2.26	0.52
1:A:1058:MET:HG2	1:A:1065:LYS:HG3	1.90	0.52
1:A:1427:ASP:O	1:B:1429:ARG:NH1	2.34	0.52
1:B:1390:HIS:O	1:B:1394:ILE:HG12	2.10	0.52
1:A:1037:ASP:O	1:A:1041:GLY:N	2.40	0.52
1:A:1321:LEU:O	1:A:1325:THR:OG1	2.18	0.52
1:A:1012:ARG:NH2	1:A:1017:GLU:OE1	2.42	0.52
1:A:487:THR:HG22	1:A:498:ALA:HA	1.93	0.51
1:A:1064:TYR:HB3	1:A:1125:GLU:HB3	1.90	0.51
1:B:1396:SER:O	1:B:1400:GLU:HG2	2.10	0.51
1:A:1072:GLY:O	1:B:1069:ARG:HG2	2.10	0.51
1:A:470:ASP:O	1:A:474:ASN:ND2	2.32	0.51
1:A:1396:SER:O	1:A:1400:GLU:HG2	2.09	0.51
1:B:1279:GLU:HA	1:B:1282:ARG:CZ	2.40	0.51
1:A:1135:LEU:HD21	1:A:1166:ASN:HB2	1.92	0.51
1:A:1282:ARG:C	1:A:1284:LYS:H	2.19	0.51
1:A:1336:ILE:HA	1:A:1344:LYS:O	2.11	0.51
1:B:1066:LYS:NZ	1:B:1125:GLU:OE2	2.25	0.50
1:A:1430:LEU:HG	1:B:1428:MET:O	2.12	0.50
1:B:592:TRP:HA	1:B:596:MET:HB2	1.94	0.50
1:B:592:TRP:O	1:B:597:ASN:N	2.44	0.50
1:B:1056:GLN:CB	1:B:1058:MET:HE3	2.42	0.50
1:B:471:ARG:HH21	2:D:14:DT:P	2.34	0.50
2:C:6:DT:H2''	2:C:7:DA:H5''	1.93	0.50
1:B:460:LYS:HB2	2:D:14:DT:O2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:ALA:O	1:B:1043:LYS:HE2	2.12	0.49
1:B:1083:ASP:OD1	1:B:1083:ASP:N	2.44	0.49
1:B:1232:ARG:O	1:B:1236:THR:OG1	2.23	0.49
1:A:606:VAL:O	7:A:1607:HOH:O	2.19	0.49
1:B:1056:GLN:HB3	1:B:1058:MET:HE3	1.94	0.49
1:B:1195:VAL:HG22	1:B:1352:LEU:HD22	1.94	0.49
1:A:421:CYS:HB2	1:A:450:ARG:O	2.12	0.49
1:A:1234:TYR:O	1:A:1347:ASN:HB2	2.11	0.49
1:A:442:SER:OG	1:B:1109:ASN:HB2	2.13	0.49
1:A:463:ASN:ND2	2:C:16:DC:OP2	2.36	0.49
1:B:1143:THR:HG22	1:B:1366:ARG:HB2	1.94	0.49
1:B:1135:LEU:HA	1:B:1162:ALA:HA	1.94	0.49
1:B:1043:LYS:NZ	2:C:6:DT:OP1	2.39	0.49
1:B:1252:ARG:HB3	1:B:1258:ARG:HG2	1.95	0.48
1:B:1114:ASP:OD1	1:B:1270:LYS:NZ	2.47	0.48
1:B:1151:ASP:OD2	7:B:1608:HOH:O	2.20	0.48
1:A:525:TYR:O	1:A:529:ARG:HB2	2.13	0.48
1:A:1013:ASN:OD1	1:A:1015:THR:N	2.43	0.48
1:A:418:LEU:HD11	1:A:453:ALA:HB1	1.96	0.48
1:B:1192:ILE:O	1:B:1196:LEU:N	2.37	0.48
1:B:1049:ILE:O	1:B:1053:LEU:HG	2.14	0.47
1:A:529:ARG:NE	7:A:1628:HOH:O	2.47	0.47
1:B:425:SER:O	1:B:428:GLU:HG2	2.14	0.47
1:A:1443:ALA:O	1:A:1447:GLU:HG3	2.14	0.47
1:B:581:LYS:N	1:B:585:GLU:OE2	2.37	0.47
1:A:1445:TYR:CE2	1:A:1449:LEU:HD11	2.50	0.47
1:A:1429:ARG:NH1	1:B:1427:ASP:HB3	2.30	0.47
1:B:423:SER:OG	1:B:428:GLU:OE2	2.32	0.47
1:A:607:LYS:HA	1:A:607:LYS:HD3	1.47	0.47
1:B:623:GLY:O	1:B:629:ARG:NH1	2.43	0.47
1:B:1368:GLN:O	1:B:1372:ARG:HG3	2.14	0.47
1:A:1042:LEU:HD13	1:A:1047:ARG:HA	1.97	0.47
1:B:1107:GLN:HB3	1:B:1125:GLU:HB2	1.96	0.46
1:A:1043:LYS:NZ	2:D:6:DT:OP1	2.33	0.46
1:A:1242:GLN:NE2	1:A:1330:SER:HB3	2.30	0.46
1:A:633:ILE:O	1:A:637:ALA:N	2.48	0.46
1:A:1043:LYS:HB2	1:A:1046:HIS:ND1	2.30	0.46
1:B:1367:THR:HG23	1:B:1455:LEU:HD22	1.96	0.46
1:B:1475:GLU:OE2	1:B:1479:ARG:NH2	2.45	0.46
1:A:1431:ARG:O	1:A:1437:GLU:HG3	2.15	0.46
1:B:1134:GLU:O	1:B:1163:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1299:ARG:HD3	1:B:1299:ARG:N	2.29	0.46
1:B:1419:GLU:O	1:B:1423:GLN:N	2.40	0.46
1:A:1075:MET:HE1	1:A:1083:ASP:HB3	1.98	0.46
1:A:1189:THR:HA	1:A:1477:ARG:HG3	1.97	0.46
1:A:506:MET:HG2	1:A:583:LEU:HD11	1.97	0.46
1:B:1280:LEU:HD22	1:B:1285:LYS:HD2	1.97	0.46
2:C:12:DC:H2'	2:C:13:DC:C6	2.50	0.46
1:A:510:ASP:OD2	7:A:1609:HOH:O	2.21	0.46
1:A:1012:ARG:NE	1:A:1017:GLU:OE1	2.44	0.46
1:A:1083:ASP:HB2	1:A:1121:MET:HE1	1.98	0.46
1:B:437:ASP:OD2	7:B:1612:HOH:O	2.21	0.46
1:B:1190:GLU:HB3	1:B:1213:ILE:HA	1.97	0.46
1:B:1242:GLN:NE2	1:B:1330:SER:HB2	2.31	0.46
1:B:1437:GLU:OE1	1:B:1440:LYS:HD3	2.16	0.46
2:D:5:DG:H2''	2:D:6:DT:H71	1.97	0.46
1:A:1027:MET:O	1:A:1031:VAL:HG22	2.16	0.45
1:A:1241:ILE:O	1:A:1330:SER:HA	2.16	0.45
1:B:1277:ILE:HG12	1:B:1325:THR:HG21	1.98	0.45
1:B:1409:GLU:HB3	7:B:1654:HOH:O	2.17	0.45
1:B:1465:LEU:HD23	7:B:1669:HOH:O	2.16	0.45
1:B:1422:ALA:O	1:B:1426:LEU:HG	2.17	0.45
1:A:1432:ARG:NH2	7:A:1649:HOH:O	2.42	0.45
1:B:1112:SER:OG	1:B:1116:ASP:OD2	2.20	0.45
1:A:1452:ILE:O	1:A:1456:GLU:HG3	2.16	0.45
1:B:1391:ILE:HD12	1:B:1394:ILE:HB	1.99	0.45
1:A:476:ASN:O	1:A:480:GLN:HG3	2.16	0.45
1:B:1279:GLU:HA	1:B:1282:ARG:NH2	2.32	0.45
1:B:1425:ILE:HA	1:B:1428:MET:HE2	1.99	0.45
1:A:1113:MET:HE2	1:A:1264:ILE:HD11	2.00	0.44
1:B:1274:ILE:HG23	1:B:1292:LEU:HD21	1.97	0.44
1:A:485:PHE:O	1:A:499:ARG:HG3	2.17	0.44
1:B:532:ILE:O	7:B:1614:HOH:O	2.21	0.44
1:B:1232:ARG:NH1	7:B:1642:HOH:O	2.41	0.44
1:B:1452:ILE:O	1:B:1456:GLU:HG3	2.18	0.44
1:A:470:ASP:OD1	1:A:470:ASP:N	2.51	0.44
1:A:1429:ARG:HA	1:B:1429:ARG:HA	2.00	0.44
1:A:1431:ARG:NH1	7:A:1670:HOH:O	2.51	0.44
1:B:1023:LEU:O	1:B:1027:MET:HG3	2.18	0.44
1:B:1244:ARG:HG2	1:B:1322:TYR:CE1	2.52	0.44
1:A:1431:ARG:HB3	1:B:1426:LEU:HB3	2.00	0.44
1:B:1229:GLY:HA3	1:B:1240:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:GLU:O	1:A:1092:ARG:HG3	2.18	0.43
1:B:1347:ASN:C	1:B:1347:ASN:OD1	2.61	0.43
1:B:1177:VAL:HG22	2:D:16:DC:H4'	2.00	0.43
1:A:1066:LYS:HD3	1:A:1125:GLU:HG2	2.00	0.43
1:B:1355:TYR:O	1:B:1358:HIS:HB3	2.18	0.43
1:A:1012:ARG:NH2	1:A:1017:GLU:HA	2.33	0.43
1:A:1192:ILE:HG21	1:A:1477:ARG:HB2	2.00	0.43
1:A:1440:LYS:HE2	1:A:1440:LYS:HB3	1.67	0.43
1:A:1085:SER:HB3	2:D:7:DA:OP2	2.19	0.43
1:B:1149:ASN:ND2	1:B:1151:ASP:OD1	2.50	0.43
1:B:1365:ARG:O	7:B:1613:HOH:O	2.21	0.43
1:A:1191:LEU:HD23	1:A:1191:LEU:HA	1.86	0.43
1:A:1376:ASP:O	1:A:1379:HIS:HB3	2.18	0.43
1:B:627:GLU:OE2	1:B:630:ARG:NH2	2.46	0.43
1:B:1381:LEU:HD23	1:B:1381:LEU:HA	1.75	0.43
1:A:481:MET:O	1:A:485:PHE:N	2.42	0.43
1:B:1251:GLU:H	1:B:1251:GLU:HG2	1.51	0.43
1:B:1293:ARG:NH1	1:B:1307:ASP:OD2	2.52	0.43
1:B:1382:GLU:OE1	7:B:1615:HOH:O	2.21	0.43
1:B:1448:LEU:HD23	1:B:1448:LEU:HA	1.79	0.43
1:A:1442:GLU:OE2	7:A:1608:HOH:O	2.20	0.43
1:B:424:LYS:O	1:B:426:PRO:HD3	2.18	0.43
1:B:587:ASN:O	1:B:590:GLN:HG3	2.19	0.43
1:B:1233:ALA:O	1:B:1237:GLY:N	2.46	0.43
1:B:1379:HIS:CD2	1:B:1421:GLN:HG3	2.53	0.43
1:A:524:PHE:O	1:A:528:MET:N	2.40	0.43
1:B:626:VAL:O	1:B:629:ARG:HB3	2.19	0.43
1:B:1040:ASP:O	1:B:1166:ASN:HB3	2.18	0.43
1:A:621:LEU:O	1:A:629:ARG:NH1	2.50	0.42
1:B:1391:ILE:O	1:B:1394:ILE:HB	2.19	0.42
1:B:427:GLU:N	1:B:427:GLU:CD	2.76	0.42
1:B:1182:ASN:ND2	1:B:1332:GLY:O	2.35	0.42
1:A:1137:ARG:HG3	7:A:1727:HOH:O	2.19	0.42
2:C:12:DC:H2'	2:C:13:DC:H6	1.85	0.42
1:B:1075:MET:HA	1:B:1079:HIS:O	2.19	0.42
1:A:1432:ARG:HD3	7:A:1670:HOH:O	2.20	0.42
1:B:1135:LEU:HG	1:B:1164:PHE:CE1	2.55	0.42
1:B:1408:MET:O	1:B:1412:GLN:HG3	2.19	0.42
1:A:1262:THR:O	1:A:1263:GLU:HG3	2.19	0.42
1:B:425:SER:OG	1:B:427:GLU:OE2	2.37	0.42
1:B:493:PHE:CE2	1:B:530:PRO:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:GLY:HA2	7:B:1711:HOH:O	2.20	0.42
1:B:1380:ILE:HG12	7:B:1607:HOH:O	2.19	0.42
2:D:6:DT:C2	2:D:7:DA:C8	3.08	0.42
2:D:12:DC:H2'	2:D:13:DC:C6	2.54	0.42
1:A:443:THR:HG22	1:A:454:ILE:HD13	2.01	0.42
1:A:530:PRO:HA	1:A:533:GLU:OE2	2.19	0.42
1:B:1140:ASN:HB2	5:B:1503:ACT:H2	2.00	0.42
1:B:1243:MET:HB2	1:B:1265:PRO:HB3	2.02	0.42
1:A:535:GLY:HA2	7:A:1607:HOH:O	2.20	0.41
1:B:1417:LEU:HD23	1:B:1417:LEU:HA	1.84	0.41
2:C:7:DA:N7	7:C:106:HOH:O	2.37	0.41
1:A:1041:GLY:HA2	1:A:1167:LEU:HD13	2.02	0.41
1:A:1296:THR:HG23	1:A:1302:VAL:HA	2.02	0.41
1:B:508:ASP:O	1:B:513:GLY:HA3	2.20	0.41
1:B:1193:ASN:HA	1:B:1196:LEU:HB2	2.02	0.41
1:A:1049:ILE:HD13	1:A:1090:MET:HB2	2.02	0.41
1:A:1161:PRO:O	1:A:1358:HIS:NE2	2.52	0.41
1:B:520:LEU:HA	1:B:520:LEU:HD23	1.67	0.41
1:B:1167:LEU:HB3	7:B:1738:HOH:O	2.20	0.41
1:B:1347:ASN:OD1	1:B:1350:GLU:HG3	2.20	0.41
2:D:6:DT:OP2	7:D:101:HOH:O	2.22	0.41
1:B:1222:GLY:C	1:B:1223:LEU:HD12	2.44	0.41
1:B:1225:LEU:HD11	1:B:1244:ARG:NE	2.35	0.41
1:A:493:PHE:CE2	1:A:530:PRO:HB2	2.55	0.41
1:B:1041:GLY:HA2	1:B:1167:LEU:HD13	2.02	0.41
1:B:1273:MET:HE2	1:B:1273:MET:HB3	1.85	0.41
1:A:1456:GLU:O	7:A:1610:HOH:O	2.22	0.41
1:B:1191:LEU:O	1:B:1195:VAL:HG23	2.21	0.41
1:B:1384:LEU:O	1:B:1388:LEU:HG	2.21	0.41
1:A:1245:SER:OG	1:A:1265:PRO:HD3	2.20	0.41
1:B:1230:ILE:HG13	7:B:1726:HOH:O	2.21	0.41
1:A:1167:LEU:N	7:A:1679:HOH:O	2.54	0.41
1:B:1064:TYR:O	1:B:1065:LYS:HD3	2.21	0.41
1:A:1079:HIS:NE2	1:A:1081:HIS:HD2	2.19	0.41
1:A:1225:LEU:HD21	1:A:1244:ARG:HD2	2.02	0.41
1:A:1327:LEU:HD23	1:A:1327:LEU:HA	1.81	0.41
1:B:535:GLY:HA3	1:B:605:GLN:NE2	2.35	0.41
1:B:1164:PHE:O	1:B:1166:ASN:N	2.54	0.41
1:B:1242:GLN:HE22	1:B:1330:SER:HB2	1.86	0.41
1:B:1363:VAL:HG21	1:B:1469:VAL:HG22	2.03	0.41
1:A:1079:HIS:CE1	1:A:1081:HIS:HD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1245:SER:HB3	1:B:1263:GLU:O	2.21	0.41
1:A:1041:GLY:HA3	1:A:1167:LEU:HA	2.02	0.40
1:A:1129:THR:OG1	1:A:1132:THR:OG1	2.37	0.40
1:A:1384:LEU:O	1:A:1388:LEU:HG	2.21	0.40
1:B:460:LYS:HA	1:B:460:LYS:HD3	1.90	0.40
2:D:13:DC:H2'	2:D:14:DT:C6	2.56	0.40
1:A:486:GLY:O	1:A:497:LYS:HB3	2.21	0.40
1:A:1242:GLN:HE22	1:A:1330:SER:HB3	1.86	0.40
1:A:1344:LYS:HZ2	1:A:1350:GLU:CD	2.27	0.40
1:A:1412:GLN:HA	1:A:1417:LEU:HB2	2.03	0.40
1:B:514:ALA:O	1:B:518:THR:HG23	2.19	0.40
1:B:639:TYR:CE1	1:B:1031:VAL:HG11	2.56	0.40
1:A:598:PRO:HA	1:A:601:ARG:NE	2.37	0.40
1:B:1113:MET:HE3	1:B:1113:MET:HB2	1.94	0.40
1:A:1067:SER:HB3	1:A:1090:MET:HE1	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1675:HOH:O	7:B:1756:HOH:O[5_664]	2.13	0.07
7:A:1738:HOH:O	7:B:1792:HOH:O[5_664]	2.17	0.03

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	666/692 (96%)	632 (95%)	32 (5%)	2 (0%)	36	34
1	B	667/692 (96%)	638 (96%)	28 (4%)	1 (0%)	48	50
All	All	1333/1384 (96%)	1270 (95%)	60 (4%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1033	ARG
1	A	1283	ASP
1	B	1033	ARG

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	574/591 (97%)	563 (98%)	11 (2%)	50	56
1	B	574/591 (97%)	564 (98%)	10 (2%)	53	60
All	All	1148/1182 (97%)	1127 (98%)	21 (2%)	51	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	LEU
1	A	431	ILE
1	A	483	THR
1	A	492	ASP
1	A	581	LYS
1	A	1010	ASN
1	A	1083	ASP
1	A	1285	LYS
1	A	1300	THR
1	A	1453	SER
1	A	1465	LEU
1	B	423	SER
1	B	427	GLU
1	B	461	ILE
1	B	503	ILE
1	B	590	GLN
1	B	595	THR
1	B	1148	ASP
1	B	1249	ILE
1	B	1350	GLU

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Mol	Chain	Res	Type
1	B	1403	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	480	GLN
1	A	1054	ASN
1	A	1056	GLN
1	A	1081	HIS
1	A	1370	ASN
1	B	1081	HIS
1	B	1107	GLN
1	B	1446	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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
6	6II	B	1504	-	30,33,33	1.84	9 (30%)	30,48,48	2.55	8 (26%)
5	ACT	B	1503	-	3,3,3	1.27	0	3,3,3	1.30	0

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
6	6II	B	1504	-	-	4/7/25/25	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1504	6II	C2-N3	3.97	1.53	1.49
6	B	1504	6II	C14-CL15	-3.11	1.68	1.74
6	B	1504	6II	C19-C20	-3.09	1.38	1.44
6	B	1504	6II	C7-C8	-2.98	1.47	1.51
6	B	1504	6II	C19-C18	-2.85	1.33	1.37
6	B	1504	6II	F27-C26	-2.74	1.29	1.36
6	B	1504	6II	C18-N17	2.71	1.37	1.34
6	B	1504	6II	C4-N3	2.44	1.52	1.49
6	B	1504	6II	O22-C23	-2.32	1.35	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1504	6II	C19-C18-N17	-7.71	112.42	124.76
6	B	1504	6II	C1-C16-N17	-7.26	100.17	112.77
6	B	1504	6II	C25-C24-C18	3.92	127.62	120.32
6	B	1504	6II	C9-C10-C6	-3.40	100.33	103.64
6	B	1504	6II	O22-C23-C29	-3.11	112.11	116.25
6	B	1504	6II	C12-C11-C9	-3.00	116.77	119.58
6	B	1504	6II	O22-C23-C24	2.57	123.91	121.57
6	B	1504	6II	C29-C23-C24	2.18	123.99	119.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1504	6II	N3-C5-C6-C10

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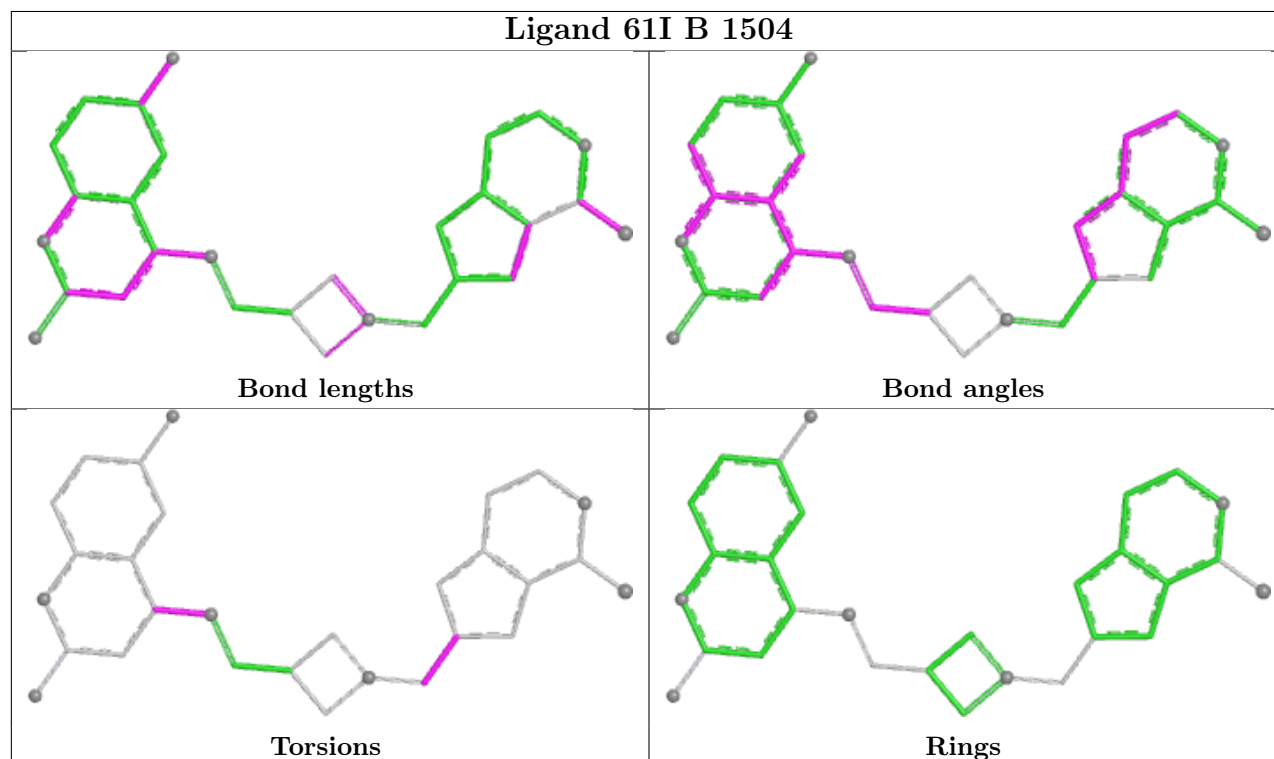
Mol	Chain	Res	Type	Atoms
6	B	1504	61I	N3-C5-C6-C7
6	B	1504	61I	C19-C18-N17-C16
6	B	1504	61I	C24-C18-N17-C16

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1503	ACT	2	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 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 [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	670/692 (96%)	-1.02	0 100 100	23, 32, 44, 54	0
1	B	671/692 (96%)	-1.02	0 100 100	23, 32, 43, 48	0
2	C	20/20 (100%)	-1.45	0 100 100	25, 30, 38, 39	0
2	D	20/20 (100%)	-1.45	0 100 100	24, 30, 40, 50	0
All	All	1381/1424 (96%)	-1.03	0 100 100	23, 32, 44, 54	0

There are no RSRZ outliers to report.

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, 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.

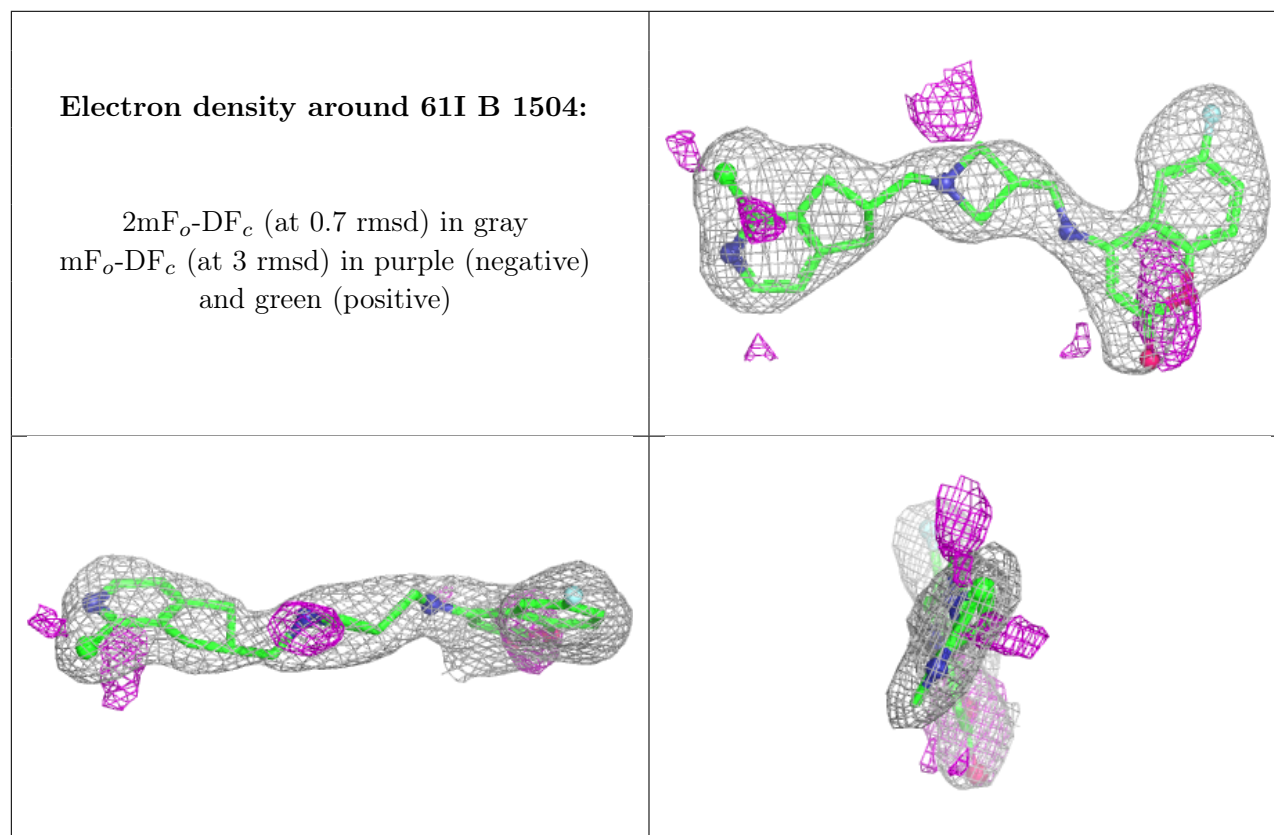
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	B	1503	4/4	0.96	0.08	32,32,34,36	0
6	61I	B	1504	29/29	0.97	0.07	30,35,39,47	0
3	MN	B	1502	1/1	0.98	0.11	46,46,46,46	0
4	CL	A	1502	1/1	0.99	0.04	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	A	1501	1/1	1.00	0.03	31,31,31,31	0
3	MN	B	1501	1/1	1.00	0.03	32,32,32,32	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.