



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:52 PM UTC

PDB ID : 4I9I / pdb_00004i9i
Title : Crystal structure of tankyrase 1 with compound 4
Authors : Huang, X.
Deposited on : 2012-12-05
Resolution : 2.40 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

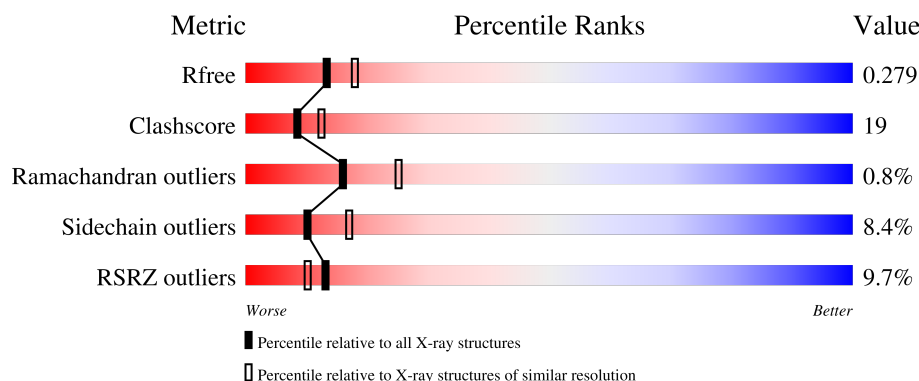
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	217	7% 64% 26% 6% ..
1	B	217	9% 63% 25% 7% ..
1	C	217	10% 57% 30% 7% ..
1	D	217	11% 53% 34% 6% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7021 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 Tankyrase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1698	1066	313	307	12			
1	B	211	Total	C	N	O	S	0	0	0
			1687	1060	310	306	11			
1	C	209	Total	C	N	O	S	0	0	0
			1675	1054	307	303	11			
1	D	206	Total	C	N	O	S	0	0	0
			1651	1038	304	298	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1315	HIS	-	expression tag	UNP O95271
A	1316	HIS	-	expression tag	UNP O95271
A	1317	HIS	-	expression tag	UNP O95271
A	1318	HIS	-	expression tag	UNP O95271
A	1319	HIS	-	expression tag	UNP O95271
A	1320	HIS	-	expression tag	UNP O95271
B	1315	HIS	-	expression tag	UNP O95271
B	1316	HIS	-	expression tag	UNP O95271
B	1317	HIS	-	expression tag	UNP O95271
B	1318	HIS	-	expression tag	UNP O95271
B	1319	HIS	-	expression tag	UNP O95271
B	1320	HIS	-	expression tag	UNP O95271
C	1315	HIS	-	expression tag	UNP O95271
C	1316	HIS	-	expression tag	UNP O95271
C	1317	HIS	-	expression tag	UNP O95271
C	1318	HIS	-	expression tag	UNP O95271
C	1319	HIS	-	expression tag	UNP O95271
C	1320	HIS	-	expression tag	UNP O95271
D	1315	HIS	-	expression tag	UNP O95271
D	1316	HIS	-	expression tag	UNP O95271
D	1317	HIS	-	expression tag	UNP O95271

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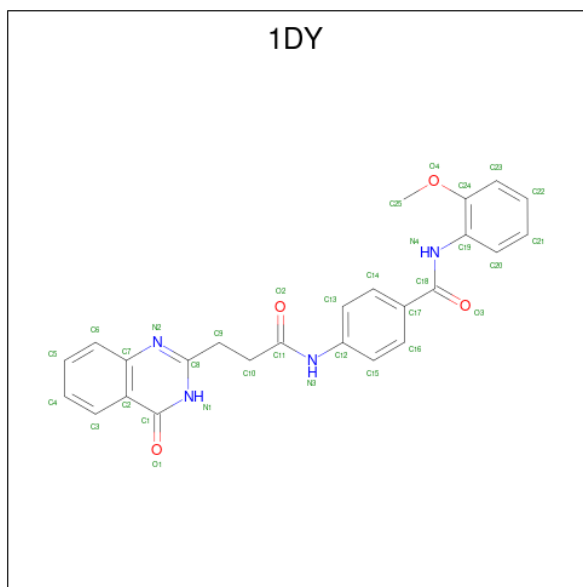
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1318	HIS	-	expression tag	UNP O95271
D	1319	HIS	-	expression tag	UNP O95271
D	1320	HIS	-	expression tag	UNP O95271

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is N-(2-methoxyphenyl)-4-{[3-(4-oxo-3,4-dihydroquinazolin-2-yl)propanoyl]amino}benzamide (CCD ID: 1DY) (formula: C₂₅H₂₂N₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 33 25 4 4	0	0
3	B	1	Total C N O 33 25 4 4	0	0
3	C	1	Total C N O 33 25 4 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			33	25	4	4		

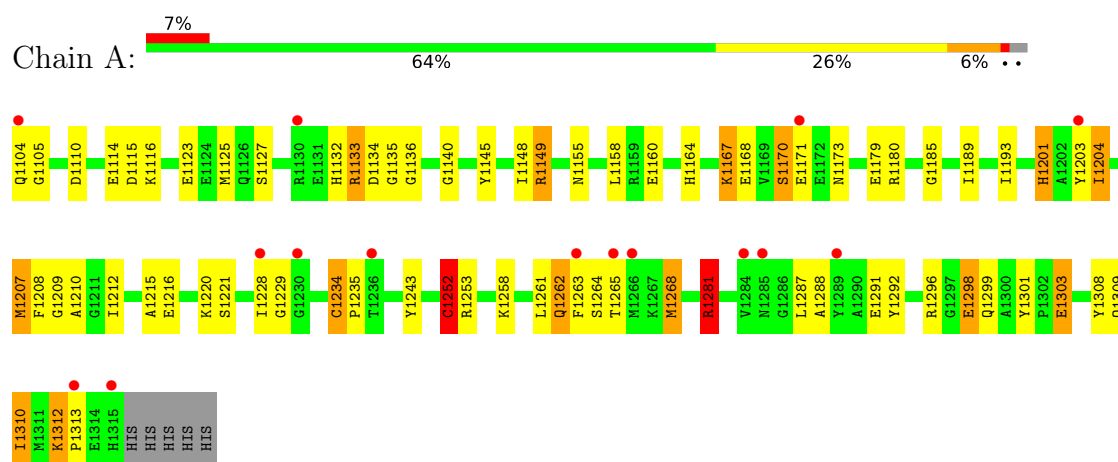
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		
4	B	36	Total	O	0	0
			36	36		
4	C	49	Total	O	0	0
			49	49		
4	D	49	Total	O	0	0
			49	49		

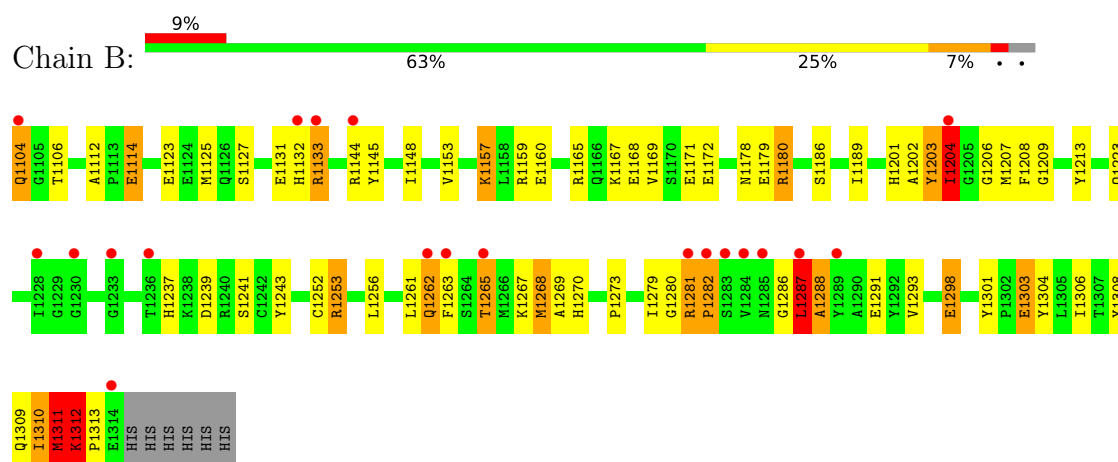
3 Residue-property plots [i](#)

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.

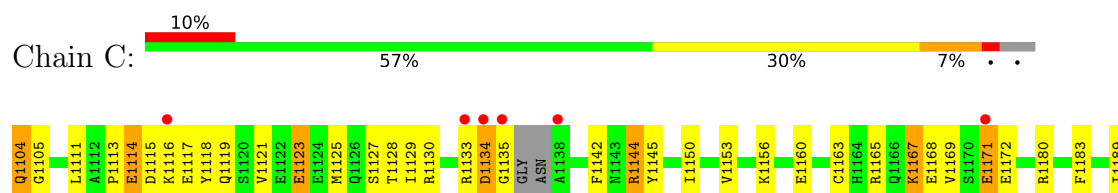
• Molecule 1: Tankyrase-1

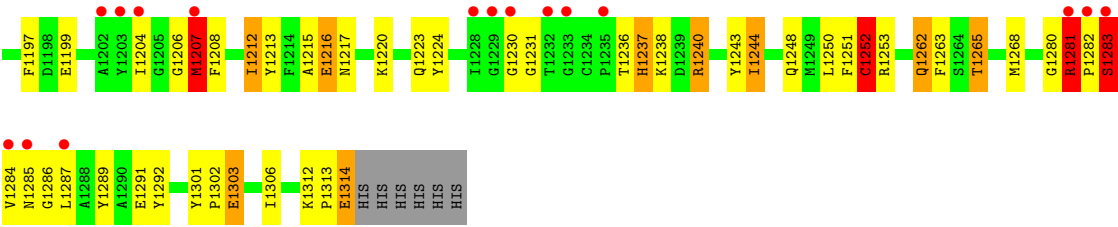


• Molecule 1: Tankyrase-1

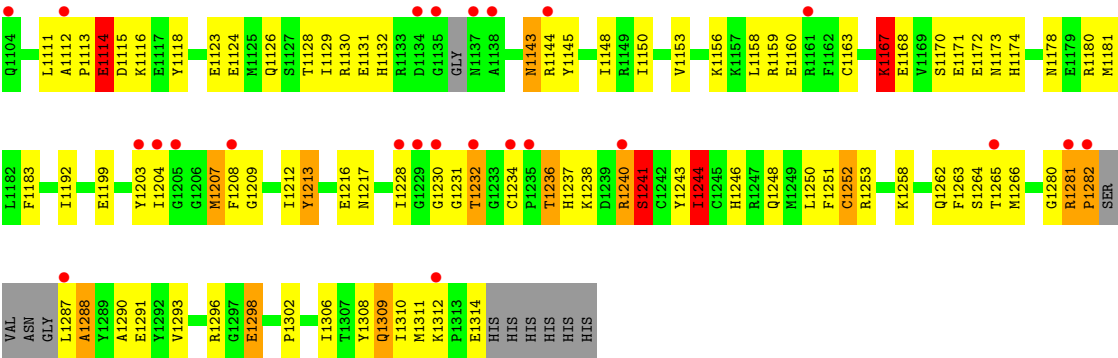


• Molecule 1: Tankyrase-1





• Molecule 1: Tankyrase-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	158.62Å 77.12Å 84.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.41	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 98.0 (50.00-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.286 0.247 , 0.279	Depositor DCC
R_{free} test set	2004 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.770	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7021	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 43.46 % 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 1.7579e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 1DY, ZN

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	0.67	2/1741 (0.1%)	1.23	19/2340 (0.8%)
1	B	0.64	1/1729 (0.1%)	1.27	23/2325 (1.0%)
1	C	0.69	2/1716 (0.1%)	1.27	20/2306 (0.9%)
1	D	0.62	1/1691 (0.1%)	1.25	25/2272 (1.1%)
All	All	0.66	6/6877 (0.1%)	1.26	87/9243 (0.9%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1207	MET	SD-CE	6.77	1.96	1.79
1	A	1228	ILE	CA-CB	6.75	1.61	1.54
1	A	1204	ILE	CA-CB	5.46	1.61	1.54
1	C	1204	ILE	CA-CB	5.25	1.62	1.54
1	D	1207	MET	SD-CE	5.07	1.92	1.79
1	B	1204	ILE	CA-CB	5.01	1.61	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1262	GLN	CB-CG-CD	-12.09	92.05	112.60
1	C	1285	ASN	N-CA-C	-11.16	99.32	113.16
1	C	1262	GLN	CB-CG-CD	-10.92	94.04	112.60
1	B	1262	GLN	CB-CG-CD	-10.84	94.16	112.60
1	D	1291	GLU	CB-CG-CD	-9.46	96.52	112.60
1	D	1168	GLU	N-CA-C	-9.30	101.22	111.36
1	B	1206	GLY	N-CA-C	9.24	122.56	111.93
1	A	1312	LYS	CA-C-N	9.07	131.18	119.84
1	A	1312	LYS	C-N-CA	9.07	131.18	119.84
1	A	1234	CYS	CA-C-N	8.99	129.57	119.32
1	A	1234	CYS	C-N-CA	8.99	129.57	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1168	GLU	N-CA-C	-8.95	101.48	111.14
1	A	1168	GLU	N-CA-C	-8.68	101.51	110.97
1	C	1133	ARG	N-CA-C	-8.47	103.07	113.41
1	B	1312	LYS	CA-C-N	8.14	128.20	119.89
1	B	1312	LYS	C-N-CA	8.14	128.20	119.89
1	B	1281	ARG	CA-C-N	8.10	129.97	119.84
1	B	1281	ARG	C-N-CA	8.10	129.97	119.84
1	A	1252	CYS	N-CA-C	7.93	122.43	110.14
1	D	1172	GLU	CB-CG-CD	-7.78	99.38	112.60
1	A	1262	GLN	N-CA-C	7.53	120.91	109.23
1	C	1281	ARG	N-CA-C	7.38	120.96	110.40
1	D	1236	THR	N-CA-C	7.33	120.32	111.82
1	C	1206	GLY	N-CA-C	7.28	120.34	112.33
1	C	1265	THR	N-CA-C	7.27	121.61	108.17
1	C	1291	GLU	CB-CG-CD	-7.09	100.55	112.60
1	D	1232	THR	N-CA-C	-7.01	101.94	111.55
1	C	1303	GLU	N-CA-C	6.97	118.53	111.07
1	D	1240	ARG	N-CA-C	-6.82	95.16	107.98
1	B	1287	LEU	N-CA-C	6.59	120.04	110.42
1	D	1132	HIS	N-CA-C	6.53	120.88	112.26
1	C	1252	CYS	N-CA-C	6.42	119.16	109.41
1	C	1172	GLU	CB-CG-CD	-6.23	102.01	112.60
1	A	1303	GLU	CB-CG-CD	-6.17	102.11	112.60
1	C	1283	SER	N-CA-C	-6.17	100.03	109.41
1	C	1216	GLU	CB-CG-CD	-6.12	102.20	112.60
1	D	1209	GLY	N-CA-C	6.11	122.49	112.84
1	A	1303	GLU	N-CA-C	6.10	118.43	111.11
1	B	1303	GLU	N-CA-C	6.08	117.91	111.28
1	A	1287	LEU	N-CA-C	6.04	118.09	110.24
1	D	1252	CYS	N-CA-C	6.03	119.38	109.85
1	D	1159	ARG	N-CA-C	-6.01	104.81	111.36
1	B	1160	GLU	CB-CG-CD	-5.84	102.67	112.60
1	B	1213	TYR	N-CA-C	5.82	119.74	109.96
1	D	1266	MET	N-CA-C	-5.82	99.75	109.24
1	A	1299	GLN	CB-CG-CD	5.77	122.41	112.60
1	A	1298	GLU	CB-CG-CD	5.70	122.29	112.60
1	D	1213	TYR	N-CA-C	5.70	119.38	110.32
1	D	1308	TYR	N-CA-C	5.64	116.00	108.38
1	B	1253	ARG	N-CA-C	-5.63	100.01	108.96
1	A	1201	HIS	N-CA-C	-5.59	104.88	112.26
1	B	1104	GLN	CB-CG-CD	-5.58	103.11	112.60
1	C	1171	GLU	N-CA-C	-5.58	104.21	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1167	LYS	CD-CE-NZ	5.57	129.73	111.90
1	D	1126	GLN	CB-CG-CD	5.57	122.06	112.60
1	D	1253	ARG	N-CA-C	-5.54	100.16	108.96
1	B	1304	TYR	N-CA-C	5.46	117.98	108.76
1	C	1213	TYR	N-CA-C	5.45	118.70	109.76
1	B	1311	MET	N-CA-C	5.45	118.36	109.59
1	C	1172	GLU	N-CA-C	5.42	119.37	112.87
1	C	1223	GLN	CB-CG-CD	-5.42	103.39	112.60
1	B	1172	GLU	CB-CG-CD	-5.41	103.40	112.60
1	A	1135	GLY	N-CA-C	-5.39	107.81	115.30
1	A	1160	GLU	CB-CG-CD	5.37	121.72	112.60
1	D	1244	ILE	CB-CA-C	-5.35	106.28	111.05
1	B	1269	ALA	N-CA-C	-5.34	107.31	113.88
1	D	1309	GLN	CB-CG-CD	-5.34	103.52	112.60
1	B	1202	ALA	N-CA-C	5.33	118.38	110.48
1	B	1253	ARG	CB-CG-CD	-5.32	99.06	111.30
1	A	1281	ARG	N-CA-C	5.30	116.50	109.93
1	D	1288	ALA	N-CA-C	-5.29	104.95	111.40
1	B	1310	ILE	N-CA-C	-5.28	100.79	108.97
1	A	1212	ILE	N-CA-C	-5.27	100.17	107.80
1	C	1251	PHE	N-CA-C	-5.26	98.81	108.02
1	C	1134	ASP	N-CA-C	5.25	117.86	110.14
1	B	1303	GLU	CB-CG-CD	-5.21	103.74	112.60
1	D	1192	ILE	N-CA-C	5.21	115.93	110.62
1	B	1252	CYS	N-CA-C	5.19	118.46	110.42
1	C	1168	GLU	N-CA-C	-5.18	105.06	111.33
1	A	1291	GLU	CB-CG-CD	-5.17	103.81	112.60
1	D	1114	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	1310	ILE	N-CA-C	-5.11	101.04	109.12
1	C	1212	ILE	N-CA-C	-5.11	101.02	108.17
1	D	1216	GLU	N-CA-C	-5.10	107.06	113.28
1	D	1251	PHE	N-CA-C	-5.09	99.12	108.02
1	D	1290	ALA	N-CA-C	-5.08	102.18	110.20
1	B	1288	ALA	N-CA-C	-5.04	106.30	112.90

There are no chirality outliers.

There are no planarity outliers.

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	1698	0	1623	53	0
1	B	1687	0	1616	72	0
1	C	1675	0	1606	80	0
1	D	1651	0	1571	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	33	0	22	3	0
3	B	33	0	22	5	0
3	C	33	0	22	2	0
3	D	33	0	22	1	0
4	A	40	0	0	4	0
4	B	36	0	0	5	0
4	C	49	0	0	3	0
4	D	49	0	0	5	0
All	All	7021	0	6504	254	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 19.

All (254) 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:C:1281:ARG:NH1	1:C:1281:ARG:HG2	1.58	1.03
1:C:1281:ARG:HG2	1:C:1281:ARG:HH11	0.86	1.01
1:B:1157:LYS:H	1:B:1157:LYS:HZ2	1.03	0.97
1:B:1203:TYR:O	1:B:1204:ILE:HG23	1.65	0.96
1:C:1144:ARG:HG2	1:C:1144:ARG:HH11	1.28	0.96
1:C:1281:ARG:HH11	1:C:1281:ARG:CG	1.79	0.94
1:D:1207:MET:HE2	1:D:1265:THR:OG1	1.74	0.88
1:C:1240:ARG:HG2	1:C:1240:ARG:HH11	1.42	0.85
1:D:1240:ARG:O	1:D:1241:SER:HB2	1.74	0.85
1:B:1180:ARG:HG2	1:B:1180:ARG:HH11	1.48	0.78
1:B:1157:LYS:HB2	1:B:1157:LYS:NZ	2.00	0.75
1:B:1157:LYS:HZ2	1:B:1157:LYS:N	1.82	0.75
1:A:1201:HIS:CD2	3:A:1402:IDY:H22	2.21	0.75
1:C:1220:LYS:HE2	1:C:1224:TYR:HE2	1.52	0.73
1:B:1148:ILE:HD11	1:B:1309:GLN:HG3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:GLU:OE2	1:A:1253:ARG:NH1	2.22	0.72
1:D:1207:MET:SD	1:D:1287:LEU:HD21	2.30	0.71
1:B:1291:GLU:HG2	3:B:1402:1DY:H4	1.72	0.71
1:B:1167:LYS:O	1:B:1171:GLU:HG3	1.91	0.70
1:A:1167:LYS:O	1:A:1171:GLU:HG3	1.91	0.70
1:B:1157:LYS:H	1:B:1157:LYS:NZ	1.87	0.69
1:C:1240:ARG:HH11	1:C:1240:ARG:CG	2.04	0.69
1:C:1199:GLU:OE1	1:C:1199:GLU:N	2.23	0.68
1:A:1148:ILE:HD11	1:A:1309:GLN:HG3	1.76	0.68
1:B:1180:ARG:HH11	1:B:1180:ARG:CG	2.06	0.67
1:A:1243:TYR:CE2	1:A:1312:LYS:HE2	2.30	0.67
1:C:1265:THR:O	1:C:1265:THR:HG22	1.95	0.67
1:C:1220:LYS:HE2	1:C:1224:TYR:CE2	2.29	0.66
1:C:1207:MET:HG3	1:C:1265:THR:OG1	1.95	0.66
1:B:1203:TYR:C	1:B:1204:ILE:HG23	2.20	0.66
1:B:1203:TYR:CB	4:B:1507:HOH:O	2.44	0.66
1:C:1314:GLU:HB2	4:C:1544:HOH:O	1.96	0.65
1:B:1180:ARG:HD3	1:C:1281:ARG:NH2	2.11	0.65
1:B:1123:GLU:OE2	1:C:1130:ARG:HA	1.96	0.64
1:D:1163:CYS:SG	4:D:1519:HOH:O	2.54	0.64
1:D:1265:THR:HG22	1:D:1265:THR:O	1.96	0.64
1:C:1189:ILE:HD12	1:C:1250:LEU:HG	1.79	0.64
1:B:1157:LYS:N	1:B:1157:LYS:HD3	2.13	0.64
1:B:1178:ASN:HD21	1:B:1180:ARG:HH12	1.44	0.63
1:B:1208:PHE:CE2	1:B:1280:GLY:HA3	2.34	0.63
1:A:1209:GLY:HA3	1:A:1268:MET:O	1.98	0.63
1:C:1144:ARG:HG2	1:C:1144:ARG:NH1	2.03	0.62
1:C:1244:ILE:HD11	1:D:1236:THR:HG21	1.80	0.62
1:C:1281:ARG:NH1	1:C:1282:PRO:HG2	2.14	0.62
1:D:1113:PRO:HA	1:D:1118:TYR:CD2	2.34	0.62
1:D:1240:ARG:O	1:D:1241:SER:CB	2.46	0.62
1:D:1128:THR:HB	1:D:1217:ASN:HA	1.82	0.61
1:A:1104:GLN:HG2	1:A:1105:GLY:N	2.14	0.61
1:B:1157:LYS:NZ	1:B:1157:LYS:CB	2.63	0.61
1:A:1262:GLN:NE2	1:A:1268:MET:HE1	2.16	0.61
1:C:1119:GLN:O	1:C:1123:GLU:HB2	2.00	0.61
1:B:1243:TYR:CE2	1:B:1312:LYS:HG2	2.35	0.61
1:D:1296:ARG:HB3	1:D:1298:GLU:OE2	2.01	0.61
1:C:1252:CYS:HB3	1:C:1301:TYR:O	2.01	0.61
1:B:1298:GLU:CD	1:B:1298:GLU:H	2.09	0.60
1:D:1232:THR:HG23	1:D:1232:THR:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:LEU:HD23	1:A:1281:ARG:HE	1.65	0.60
1:B:1208:PHE:CZ	1:B:1280:GLY:HA3	2.36	0.60
1:C:1180:ARG:HH11	1:C:1180:ARG:HG3	1.66	0.60
1:B:1157:LYS:HB2	1:B:1157:LYS:HZ3	1.64	0.60
1:D:1144:ARG:HG2	1:D:1145:TYR:N	2.16	0.60
1:B:1207:MET:HG2	1:B:1265:THR:OG1	2.01	0.59
1:A:1148:ILE:O	1:A:1149:ARG:HB3	2.00	0.59
1:A:1207:MET:HG3	1:A:1265:THR:OG1	2.03	0.59
1:A:1104:GLN:HG2	1:A:1105:GLY:H	1.65	0.59
1:D:1143:ASN:OD1	1:D:1143:ASN:O	2.20	0.59
1:C:1263:PHE:N	1:C:1263:PHE:CD2	2.70	0.59
1:B:1144:ARG:HD3	1:B:1311:MET:HE2	1.85	0.58
1:D:1148:ILE:HD11	1:D:1309:GLN:HG3	1.85	0.58
1:A:1132:HIS:C	1:A:1134:ASP:H	2.10	0.57
1:A:1262:GLN:HE21	1:A:1268:MET:HE1	1.68	0.57
1:B:1180:ARG:HG3	1:B:1256:LEU:HD12	1.87	0.57
1:C:1281:ARG:NH1	1:C:1281:ARG:CG	2.43	0.57
1:B:1265:THR:HG22	1:B:1265:THR:O	2.04	0.57
1:A:1104:GLN:CG	1:A:1105:GLY:N	2.68	0.57
1:A:1203:TYR:O	1:A:1210:ALA:HA	2.05	0.57
1:A:1133:ARG:CZ	1:A:1288:ALA:HB2	2.35	0.57
1:B:1144:ARG:HG2	1:B:1145:TYR:N	2.19	0.57
1:B:1179:GLU:OE2	1:B:1253:ARG:HD3	2.05	0.57
1:B:1180:ARG:CG	1:B:1180:ARG:NH1	2.65	0.57
1:B:1203:TYR:O	1:B:1204:ILE:CG2	2.48	0.56
1:B:1112:ALA:HB1	1:B:1114:GLU:OE2	2.06	0.56
1:B:1133:ARG:NE	1:B:1288:ALA:HB2	2.21	0.56
1:C:1128:THR:HB	1:C:1217:ASN:HA	1.88	0.56
1:D:1228:ILE:C	1:D:1230:GLY:H	2.14	0.56
1:D:1212:ILE:HG23	3:D:1402:1DY:H13	1.87	0.56
1:B:1201:HIS:CD2	3:B:1402:1DY:H22	2.42	0.55
1:D:1199:GLU:H	1:D:1199:GLU:CD	2.13	0.55
1:B:1253:ARG:HG3	1:B:1303:GLU:HG3	1.87	0.55
1:C:1197:PHE:HB3	1:C:1212:ILE:HD13	1.89	0.54
1:B:1279:ILE:HG22	1:B:1281:ARG:HG2	1.90	0.54
1:C:1237:HIS:O	1:C:1238:LYS:C	2.49	0.54
1:C:1240:ARG:CG	1:C:1240:ARG:NH1	2.68	0.54
1:C:1153:VAL:HB	1:C:1302:PRO:O	2.08	0.54
1:C:1129:ILE:HD11	1:C:1145:TYR:CE2	2.43	0.54
1:A:1203:TYR:CB	4:A:1503:HOH:O	2.57	0.53
1:C:1114:GLU:CD	1:C:1114:GLU:H	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1129:ILE:HD11	1:D:1145:TYR:CE2	2.43	0.53
1:B:1157:LYS:HZ2	1:B:1157:LYS:HB2	1.72	0.53
1:C:1115:ASP:C	1:C:1115:ASP:OD1	2.52	0.53
1:A:1132:HIS:C	1:A:1134:ASP:N	2.67	0.53
1:A:1263:PHE:N	1:A:1263:PHE:CD2	2.77	0.52
1:C:1243:TYR:CE2	1:C:1312:LYS:HG3	2.44	0.52
1:C:1180:ARG:NH2	1:C:1216:GLU:OE1	2.42	0.52
1:A:1173:ASN:ND2	1:A:1258:LYS:HB2	2.24	0.52
1:C:1134:ASP:HB2	1:C:1289:TYR:HE1	1.75	0.52
1:D:1243:TYR:CD2	1:D:1312:LYS:HD3	2.45	0.52
1:C:1281:ARG:NH2	4:C:1549:HOH:O	2.43	0.51
1:D:1180:ARG:NE	4:D:1532:HOH:O	2.32	0.51
1:A:1180:ARG:NH2	1:A:1216:GLU:OE1	2.43	0.51
1:B:1132:HIS:CD2	1:B:1223:GLN:HE21	2.28	0.51
1:D:1232:THR:O	1:D:1238:LYS:HA	2.10	0.51
1:D:1234:CYS:SG	1:D:1237:HIS:N	2.83	0.51
1:A:1123:GLU:O	1:A:1127:SER:OG	2.28	0.51
1:C:1134:ASP:CG	1:C:1135:GLY:H	2.19	0.51
1:A:1164:HIS:CD2	4:A:1539:HOH:O	2.63	0.51
1:C:1253:ARG:HG3	1:C:1303:GLU:HG3	1.92	0.51
1:C:1115:ASP:OD1	1:C:1116:LYS:N	2.44	0.51
1:C:1237:HIS:CD2	1:D:1237:HIS:CD2	2.99	0.51
1:A:1207:MET:HB3	1:A:1208:PHE:CD2	2.45	0.50
1:D:1144:ARG:HD3	1:D:1311:MET:SD	2.51	0.50
1:A:1115:ASP:OD1	1:A:1116:LYS:N	2.44	0.50
1:A:1132:HIS:O	1:A:1134:ASP:N	2.45	0.50
1:A:1155:ASN:HB3	1:A:1158:LEU:HB2	1.93	0.50
1:C:1281:ARG:HH12	1:C:1282:PRO:HG2	1.76	0.50
1:A:1265:THR:O	1:A:1265:THR:HG22	2.11	0.50
1:B:1157:LYS:HZ2	1:B:1157:LYS:CB	2.24	0.50
1:C:1282:PRO:HA	1:C:1287:LEU:HB2	1.93	0.50
1:C:1230:GLY:O	1:C:1231:GLY:C	2.55	0.50
1:C:1113:PRO:HA	1:C:1118:TYR:CG	2.46	0.50
1:C:1113:PRO:HA	1:C:1118:TYR:CD2	2.47	0.49
1:D:1112:ALA:O	1:D:1115:ASP:HB2	2.12	0.49
1:C:1283:SER:HB3	1:C:1286:GLY:HA3	1.94	0.49
1:B:1291:GLU:HG2	3:B:1402:1DY:C5	2.43	0.49
1:C:1142:PHE:HA	1:C:1313:PRO:HG3	1.93	0.49
1:C:1292:TYR:CD2	1:C:1292:TYR:N	2.81	0.49
1:D:1113:PRO:HA	1:D:1118:TYR:CG	2.48	0.49
1:B:1239:ASP:OD1	1:B:1239:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1234:CYS:SG	1:D:1238:LYS:N	2.86	0.49
1:C:1281:ARG:CG	1:C:1282:PRO:HD2	2.43	0.48
1:D:1129:ILE:HD11	1:D:1145:TYR:CD2	2.49	0.48
1:D:1167:LYS:O	1:D:1167:LYS:HG3	2.13	0.48
1:B:1144:ARG:HG2	1:B:1145:TYR:H	1.79	0.48
1:B:1273:PRO:HD2	4:B:1531:HOH:O	2.13	0.48
1:C:1144:ARG:NH1	1:C:1144:ARG:CG	2.76	0.48
1:A:1253:ARG:HG3	1:A:1303:GLU:HG3	1.96	0.48
1:C:1134:ASP:CG	1:C:1135:GLY:N	2.72	0.48
1:A:1167:LYS:HA	1:A:1170:SER:HB2	1.95	0.48
1:C:1129:ILE:HD11	1:C:1145:TYR:CD2	2.49	0.48
1:D:1213:TYR:CD1	1:D:1293:VAL:HG22	2.50	0.47
1:B:1133:ARG:NH1	1:B:1286:GLY:O	2.48	0.47
1:B:1133:ARG:CZ	1:B:1288:ALA:HB2	2.44	0.47
1:D:1180:ARG:HG3	1:D:1180:ARG:HH11	1.80	0.47
1:C:1156:LYS:O	1:C:1160:GLU:HG3	2.14	0.47
1:C:1283:SER:CB	1:C:1286:GLY:HA3	2.45	0.47
1:D:1180:ARG:HG3	4:D:1544:HOH:O	2.15	0.47
1:B:1270:HIS:HD2	4:B:1516:HOH:O	1.97	0.47
1:C:1167:LYS:HE3	1:C:1167:LYS:HB3	1.77	0.47
1:B:1243:TYR:CD1	1:B:1310:ILE:HG13	2.49	0.46
1:B:1239:ASP:OD1	1:B:1241:SER:N	2.31	0.46
1:C:1281:ARG:HG2	1:C:1282:PRO:HD2	1.98	0.46
1:D:1112:ALA:HB1	1:D:1114:GLU:OE2	2.16	0.46
1:B:1268:MET:HE3	1:B:1268:MET:HB2	1.84	0.46
1:A:1215:ALA:HB2	3:A:1402:1DY:H3	1.98	0.46
1:C:1215:ALA:HB2	3:C:1402:1DY:H3	1.98	0.46
1:D:1263:PHE:N	1:D:1263:PHE:CD2	2.83	0.46
1:B:1106:THR:HG21	1:B:1153:VAL:HG13	1.96	0.46
1:A:1268:MET:HE3	1:A:1268:MET:HB2	1.61	0.46
1:B:1179:GLU:CD	1:B:1253:ARG:HD3	2.41	0.45
1:B:1267:LYS:HB2	4:B:1533:HOH:O	2.15	0.45
1:B:1301:TYR:HD2	1:B:1303:GLU:HG2	1.82	0.45
1:C:1114:GLU:C	1:C:1119:GLN:HE21	2.24	0.45
1:C:1207:MET:HB3	1:C:1208:PHE:CE2	2.51	0.45
1:C:1236:THR:HB	1:C:1237:HIS:CE1	2.51	0.45
1:D:1111:LEU:HD12	1:D:1150:ILE:HG22	1.99	0.45
1:B:1263:PHE:N	1:B:1263:PHE:CD2	2.84	0.45
1:C:1248:GLN:HA	1:C:1306:ILE:O	2.15	0.45
1:A:1207:MET:HB3	1:A:1208:PHE:CE2	2.52	0.45
1:D:1144:ARG:HG2	1:D:1145:TYR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1183:PHE:HA	1:D:1250:LEU:O	2.16	0.45
1:B:1127:SER:HB2	1:C:1127:SER:O	2.16	0.45
1:B:1243:TYR:HD1	1:B:1310:ILE:O	2.00	0.45
1:B:1262:GLN:HE21	1:B:1262:GLN:HB3	1.29	0.45
1:C:1114:GLU:O	1:C:1119:GLN:NE2	2.50	0.45
1:A:1125:MET:HE2	1:A:1145:TYR:CD2	2.52	0.45
1:D:1111:LEU:HD12	1:D:1150:ILE:CG2	2.47	0.45
1:D:1153:VAL:HB	1:D:1302:PRO:O	2.17	0.45
1:D:1248:GLN:HA	1:D:1306:ILE:O	2.17	0.44
1:D:1310:ILE:O	1:D:1310:ILE:HG13	2.17	0.44
1:A:1243:TYR:CD1	1:A:1310:ILE:HG13	2.53	0.44
1:C:1281:ARG:NH1	1:C:1282:PRO:CG	2.78	0.44
1:C:1281:ARG:HH11	1:C:1282:PRO:HD2	1.82	0.44
1:B:1125:MET:HE1	1:B:1308:TYR:CG	2.51	0.44
1:B:1186:SER:O	1:B:1189:ILE:HG12	2.17	0.44
1:C:1262:GLN:O	1:C:1280:GLY:HA2	2.18	0.44
1:D:1207:MET:CE	1:D:1265:THR:OG1	2.58	0.44
1:D:1113:PRO:HB3	1:D:1118:TYR:CZ	2.53	0.43
1:C:1165:ARG:O	1:C:1169:VAL:HG23	2.19	0.43
1:D:1208:PHE:CE2	1:D:1280:GLY:HA3	2.54	0.43
1:D:1281:ARG:NH1	4:D:1535:HOH:O	2.52	0.43
1:C:1134:ASP:HB2	1:C:1289:TYR:CE1	2.53	0.43
1:C:1104:GLN:HG2	1:C:1105:GLY:N	2.29	0.43
1:C:1180:ARG:HH11	1:C:1180:ARG:CG	2.31	0.43
1:D:1143:ASN:OD1	1:D:1143:ASN:C	2.62	0.43
1:A:1136:GLY:O	1:A:1140:GLY:N	2.52	0.43
1:A:1185:GLY:N	1:A:1221:SER:HB3	2.34	0.43
1:D:1181:MET:HA	1:D:1252:CYS:O	2.18	0.43
1:A:1252:CYS:HB3	1:A:1301:TYR:O	2.19	0.42
1:B:1159:ARG:NH1	4:B:1510:HOH:O	2.52	0.42
1:D:1244:ILE:O	1:D:1246:HIS:HD2	2.02	0.42
1:A:1189:ILE:O	1:A:1193:ILE:HG12	2.18	0.42
1:C:1117:GLU:O	1:C:1121:VAL:HG23	2.19	0.42
1:D:1156:LYS:O	1:D:1160:GLU:HG3	2.19	0.42
1:D:1265:THR:O	1:D:1265:THR:CG2	2.67	0.42
1:A:1201:HIS:CG	3:A:1402:1DY:H22	2.53	0.42
1:A:1220:LYS:HA	1:A:1220:LYS:HD2	1.85	0.42
1:A:1312:LYS:HA	1:A:1313:PRO:HD3	1.71	0.42
1:B:1165:ARG:O	1:B:1169:VAL:HG23	2.19	0.42
1:C:1111:LEU:HD12	1:C:1150:ILE:CG2	2.49	0.42
1:A:1180:ARG:NH1	1:A:1292:TYR:OH	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1229:GLY:N	4:A:1515:HOH:O	2.53	0.42
1:B:1291:GLU:CG	3:B:1402:1DY:H4	2.46	0.42
1:D:1174:HIS:CD2	1:D:1174:HIS:N	2.87	0.42
1:A:1179:GLU:CD	1:A:1253:ARG:HH11	2.27	0.42
1:B:1243:TYR:HD1	1:B:1310:ILE:HG13	1.84	0.42
1:B:1261:LEU:HG	1:B:1281:ARG:HD2	2.01	0.42
1:C:1207:MET:O	1:C:1265:THR:HG23	2.20	0.42
1:C:1163:CYS:SG	4:C:1531:HOH:O	2.62	0.42
1:A:1204:ILE:CG2	4:A:1520:HOH:O	2.67	0.42
1:B:1157:LYS:N	1:B:1157:LYS:CD	2.83	0.42
1:B:1209:GLY:HA3	1:B:1268:MET:O	2.20	0.42
1:C:1167:LYS:O	1:C:1171:GLU:HG3	2.20	0.41
1:A:1148:ILE:CD1	1:A:1309:GLN:HG3	2.48	0.41
1:B:1180:ARG:CZ	1:C:1281:ARG:HE	2.33	0.41
1:D:1207:MET:SD	1:D:1287:LEU:CD2	3.06	0.41
1:A:1296:ARG:HB3	1:A:1298:GLU:OE2	2.21	0.41
1:D:1288:ALA:HB2	4:D:1528:HOH:O	2.20	0.41
1:A:1133:ARG:HE	1:A:1133:ARG:HB3	1.46	0.41
1:D:1230:GLY:O	1:D:1231:GLY:C	2.63	0.41
1:C:1237:HIS:ND1	1:C:1237:HIS:N	2.69	0.41
1:A:1312:LYS:HD2	1:B:1237:HIS:CD2	2.56	0.41
1:C:1125:MET:HA	1:C:1183:PHE:CZ	2.56	0.41
1:D:1282:PRO:HA	1:D:1287:LEU:HB2	2.02	0.41
3:B:1402:1DY:H16	3:B:1402:1DY:O3	2.21	0.41
1:C:1253:ARG:HH11	1:C:1253:ARG:HD3	1.70	0.41
1:B:1125:MET:SD	1:B:1306:ILE:HG21	2.61	0.40
1:C:1212:ILE:HG23	3:C:1402:1DY:H13	2.03	0.40
1:A:1234:CYS:HA	1:A:1235:PRO:HD3	1.75	0.40
1:D:1173:ASN:ND2	1:D:1258:LYS:HB2	2.36	0.40
1:B:1207:MET:HE1	1:B:1287:LEU:HG	2.03	0.40
1:B:1133:ARG:HE	1:B:1133:ARG:HB3	1.77	0.40
1:B:1180:ARG:HD3	1:C:1281:ARG:HH21	1.85	0.40
1:A:1125:MET:HE1	1:A:1308:TYR:CG	2.56	0.40
1:B:1312:LYS:HA	1:B:1313:PRO:HD3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	210/217 (97%)	204 (97%)	5 (2%)	1 (0%)	24	37
1	B	209/217 (96%)	200 (96%)	6 (3%)	3 (1%)	9	13
1	C	205/217 (94%)	194 (95%)	11 (5%)	0	100	100
1	D	200/217 (92%)	191 (96%)	6 (3%)	3 (2%)	8	12
All	All	824/868 (95%)	789 (96%)	28 (3%)	7 (1%)	16	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1203	TYR
1	B	1204	ILE
1	D	1203	TYR
1	D	1204	ILE
1	D	1241	SER
1	A	1133	ARG
1	B	1282	PRO

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	177/185 (96%)	167 (94%)	10 (6%)	19	33
1	B	176/185 (95%)	161 (92%)	15 (8%)	10	16
1	C	175/185 (95%)	160 (91%)	15 (9%)	10	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	171/185 (92%)	152 (89%)	19 (11%)	6	9
All	All	699/740 (94%)	640 (92%)	59 (8%)	10	17

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1110	ASP
1	A	1114	GLU
1	A	1149	ARG
1	A	1167	LYS
1	A	1170	SER
1	A	1207	MET
1	A	1252	CYS
1	A	1264	SER
1	A	1268	MET
1	A	1281	ARG
1	B	1104	GLN
1	B	1114	GLU
1	B	1131	GLU
1	B	1133	ARG
1	B	1157	LYS
1	B	1180	ARG
1	B	1204	ILE
1	B	1265	THR
1	B	1268	MET
1	B	1282	PRO
1	B	1287	LEU
1	B	1293	VAL
1	B	1298	GLU
1	B	1311	MET
1	B	1312	LYS
1	C	1104	GLN
1	C	1114	GLU
1	C	1123	GLU
1	C	1144	ARG
1	C	1167	LYS
1	C	1207	MET
1	C	1237	HIS
1	C	1240	ARG
1	C	1244	ILE
1	C	1252	CYS
1	C	1268	MET

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Mol	Chain	Res	Type
1	C	1281	ARG
1	C	1283	SER
1	C	1284	VAL
1	C	1314	GLU
1	D	1114	GLU
1	D	1116	LYS
1	D	1123	GLU
1	D	1124	GLU
1	D	1130	ARG
1	D	1131	GLU
1	D	1143	ASN
1	D	1158	LEU
1	D	1167	LYS
1	D	1170	SER
1	D	1171	GLU
1	D	1178	ASN
1	D	1241	SER
1	D	1244	ILE
1	D	1264	SER
1	D	1281	ARG
1	D	1282	PRO
1	D	1298	GLU
1	D	1314	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1146	ASN
1	A	1166	GLN
1	A	1173	ASN
1	A	1177	HIS
1	A	1190	ASN
1	A	1201	HIS
1	A	1248	GLN
1	A	1309	GLN
1	B	1104	GLN
1	B	1166	GLN
1	B	1177	HIS
1	B	1178	ASN
1	B	1201	HIS
1	B	1217	ASN
1	B	1223	GLN

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Mol	Chain	Res	Type
1	B	1262	GLN
1	C	1119	GLN
1	C	1151	GLN
1	C	1166	GLN
1	C	1173	ASN
1	C	1190	ASN
1	C	1223	GLN
1	C	1262	GLN
1	D	1119	GLN
1	D	1166	GLN
1	D	1173	ASN
1	D	1223	GLN
1	D	1246	HIS
1	D	1248	GLN
1	D	1262	GLN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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
3	1DY	B	1402	-	34,36,36	2.57	20 (58%)	46,49,49	2.02	14 (30%)
3	1DY	A	1402	-	34,36,36	2.52	19 (55%)	46,49,49	2.17	11 (23%)
3	1DY	D	1402	-	34,36,36	2.71	20 (58%)	46,49,49	1.68	12 (26%)
3	1DY	C	1402	-	34,36,36	2.53	21 (61%)	46,49,49	1.69	11 (23%)

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
3	1DY	B	1402	-	-	3/19/19/19	0/4/4/4
3	1DY	A	1402	-	-	3/19/19/19	0/4/4/4
3	1DY	D	1402	-	-	0/19/19/19	0/4/4/4
3	1DY	C	1402	-	-	2/19/19/19	0/4/4/4

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1402	1DY	C14-C17	5.11	1.47	1.39
3	B	1402	1DY	C2-C7	4.65	1.46	1.40
3	A	1402	1DY	C14-C17	4.61	1.46	1.39
3	C	1402	1DY	C14-C13	4.57	1.46	1.38
3	A	1402	1DY	C21-C20	4.55	1.46	1.38
3	D	1402	1DY	C2-C7	4.43	1.46	1.40
3	D	1402	1DY	C14-C17	4.33	1.46	1.39
3	D	1402	1DY	C6-C7	4.31	1.46	1.40
3	B	1402	1DY	C14-C17	4.21	1.45	1.39
3	A	1402	1DY	C14-C13	4.20	1.45	1.38
3	D	1402	1DY	C14-C13	4.18	1.45	1.38
3	B	1402	1DY	C21-C20	4.15	1.46	1.38
3	B	1402	1DY	C14-C13	4.14	1.45	1.38
3	D	1402	1DY	C16-C15	4.12	1.45	1.38
3	D	1402	1DY	C15-C12	3.94	1.45	1.39
3	D	1402	1DY	C5-C6	3.94	1.45	1.38
3	B	1402	1DY	C15-C12	3.92	1.45	1.39
3	D	1402	1DY	C4-C3	3.83	1.45	1.38
3	A	1402	1DY	C15-C12	3.74	1.45	1.39
3	C	1402	1DY	C16-C15	3.66	1.44	1.38
3	A	1402	1DY	C23-C24	3.50	1.46	1.39
3	D	1402	1DY	C5-C4	3.49	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1402	1DY	C5-C6	3.40	1.44	1.38
3	B	1402	1DY	C22-C23	3.36	1.44	1.38
3	C	1402	1DY	C16-C17	3.29	1.44	1.39
3	D	1402	1DY	C16-C17	3.29	1.44	1.39
3	A	1402	1DY	C4-C3	3.28	1.44	1.38
3	C	1402	1DY	C13-C12	3.27	1.44	1.39
3	C	1402	1DY	C23-C24	3.27	1.46	1.39
3	C	1402	1DY	C6-C7	3.23	1.45	1.40
3	A	1402	1DY	C22-C23	3.21	1.44	1.38
3	A	1402	1DY	C2-C7	3.18	1.44	1.40
3	C	1402	1DY	C12-N3	-3.18	1.35	1.41
3	B	1402	1DY	C5-C4	3.17	1.45	1.38
3	D	1402	1DY	C12-N3	-3.17	1.35	1.41
3	B	1402	1DY	C20-C19	3.16	1.44	1.39
3	C	1402	1DY	C21-C20	3.10	1.44	1.38
3	D	1402	1DY	C21-C20	3.08	1.44	1.38
3	B	1402	1DY	C4-C3	3.08	1.44	1.38
3	C	1402	1DY	C5-C4	3.08	1.45	1.38
3	C	1402	1DY	C15-C12	3.07	1.44	1.39
3	B	1402	1DY	C7-N2	-3.05	1.33	1.39
3	B	1402	1DY	C16-C17	3.05	1.44	1.39
3	A	1402	1DY	C1-N1	-3.04	1.33	1.37
3	B	1402	1DY	C16-C15	3.02	1.43	1.38
3	A	1402	1DY	C5-C6	3.00	1.44	1.38
3	D	1402	1DY	C13-C12	2.99	1.44	1.39
3	C	1402	1DY	C20-C19	2.97	1.44	1.39
3	A	1402	1DY	C20-C19	2.96	1.44	1.39
3	A	1402	1DY	C22-C21	2.90	1.44	1.38
3	A	1402	1DY	C6-C7	2.90	1.44	1.40
3	B	1402	1DY	C23-C24	2.90	1.45	1.39
3	B	1402	1DY	C12-N3	-2.81	1.36	1.41
3	D	1402	1DY	C20-C19	2.81	1.44	1.39
3	A	1402	1DY	C13-C12	2.71	1.43	1.39
3	D	1402	1DY	C22-C21	2.70	1.44	1.38
3	A	1402	1DY	C12-N3	-2.70	1.36	1.41
3	D	1402	1DY	C22-C23	2.66	1.43	1.38
3	C	1402	1DY	C2-C1	-2.60	1.42	1.47
3	B	1402	1DY	C3-C2	2.56	1.43	1.39
3	D	1402	1DY	C23-C24	2.54	1.44	1.39
3	A	1402	1DY	C16-C17	2.52	1.43	1.39
3	A	1402	1DY	C5-C4	2.50	1.43	1.38
3	C	1402	1DY	C2-C7	2.48	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1402	1DY	C13-C12	2.46	1.43	1.39
3	B	1402	1DY	C22-C21	2.44	1.43	1.38
3	D	1402	1DY	C3-C2	2.44	1.43	1.39
3	B	1402	1DY	C5-C6	2.42	1.43	1.38
3	A	1402	1DY	C16-C15	2.34	1.42	1.38
3	A	1402	1DY	C7-N2	-2.30	1.35	1.39
3	C	1402	1DY	C9-C8	2.23	1.53	1.49
3	D	1402	1DY	C7-N2	-2.21	1.35	1.39
3	D	1402	1DY	C9-C8	2.21	1.53	1.49
3	C	1402	1DY	C22-C21	2.19	1.43	1.38
3	B	1402	1DY	C1-N1	-2.19	1.34	1.37
3	C	1402	1DY	C19-N4	-2.18	1.37	1.41
3	C	1402	1DY	C4-C3	2.18	1.42	1.38
3	B	1402	1DY	C6-C7	2.18	1.43	1.40
3	C	1402	1DY	C22-C23	2.16	1.42	1.38
3	C	1402	1DY	C19-C24	2.16	1.44	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	1DY	O4-C24-C19	-7.47	105.51	114.81
3	B	1402	1DY	C1-N1-C8	5.92	127.32	123.90
3	A	1402	1DY	C10-C9-C8	-5.39	107.00	112.55
3	D	1402	1DY	C1-N1-C8	4.43	126.46	123.90
3	A	1402	1DY	C16-C17-C14	4.32	124.06	118.57
3	A	1402	1DY	O4-C24-C23	3.98	131.02	124.30
3	B	1402	1DY	C16-C17-C14	3.96	123.61	118.57
3	C	1402	1DY	O1-C1-N1	3.89	125.23	120.62
3	B	1402	1DY	C6-C7-C2	3.71	122.79	119.14
3	A	1402	1DY	C2-C7-N2	-3.64	118.75	122.41
3	A	1402	1DY	C15-C16-C17	-3.59	116.97	120.80
3	C	1402	1DY	C2-C7-N2	-3.52	118.88	122.41
3	B	1402	1DY	O4-C24-C19	-3.47	110.50	114.81
3	D	1402	1DY	C16-C17-C14	3.32	122.80	118.57
3	C	1402	1DY	C15-C12-C13	3.31	123.44	119.04
3	C	1402	1DY	N1-C8-N2	-3.29	118.91	123.08
3	D	1402	1DY	C25-O4-C24	3.21	122.22	117.51
3	B	1402	1DY	C15-C12-C13	3.13	123.19	119.04
3	D	1402	1DY	C15-C12-C13	3.09	123.15	119.04
3	B	1402	1DY	N1-C8-N2	-3.05	119.21	123.08
3	D	1402	1DY	C6-C7-C2	3.04	122.13	119.14
3	D	1402	1DY	C2-C7-N2	-2.98	119.42	122.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1402	1DY	C15-C12-C13	2.80	122.76	119.04
3	B	1402	1DY	C15-C16-C17	-2.79	117.81	120.80
3	C	1402	1DY	C1-N1-C8	2.73	125.48	123.90
3	A	1402	1DY	C6-C7-C2	2.70	121.80	119.14
3	C	1402	1DY	C3-C2-C7	2.67	122.83	119.78
3	D	1402	1DY	N1-C8-N2	-2.63	119.74	123.08
3	C	1402	1DY	C16-C17-C14	2.59	121.86	118.57
3	B	1402	1DY	C2-C7-N2	-2.53	119.87	122.41
3	C	1402	1DY	C10-C9-C8	-2.52	109.95	112.55
3	B	1402	1DY	C4-C3-C2	-2.47	115.33	119.80
3	B	1402	1DY	C4-C5-C6	2.47	123.28	120.24
3	C	1402	1DY	C12-N3-C11	2.46	131.88	127.52
3	B	1402	1DY	C13-C14-C17	-2.45	118.18	120.80
3	D	1402	1DY	C2-C1-N1	-2.41	112.39	114.93
3	A	1402	1DY	C13-C14-C17	-2.41	118.23	120.80
3	A	1402	1DY	C14-C13-C12	-2.41	117.53	120.30
3	B	1402	1DY	C5-C6-C7	-2.32	114.71	118.97
3	A	1402	1DY	C23-C24-C19	2.28	123.47	120.39
3	D	1402	1DY	C13-C12-N3	-2.18	113.10	120.41
3	D	1402	1DY	O1-C1-C2	2.17	127.14	123.27
3	B	1402	1DY	O4-C24-C23	2.13	127.90	124.30
3	C	1402	1DY	O1-C1-C2	-2.09	119.53	123.27
3	D	1402	1DY	C15-C16-C17	-2.07	118.58	120.80
3	C	1402	1DY	C14-C13-C12	-2.02	117.97	120.30
3	B	1402	1DY	C10-C9-C8	-2.01	110.48	112.55
3	D	1402	1DY	C10-C9-C8	2.01	114.62	112.55

There are no chirality outliers.

All (8) torsion outliers are listed below:

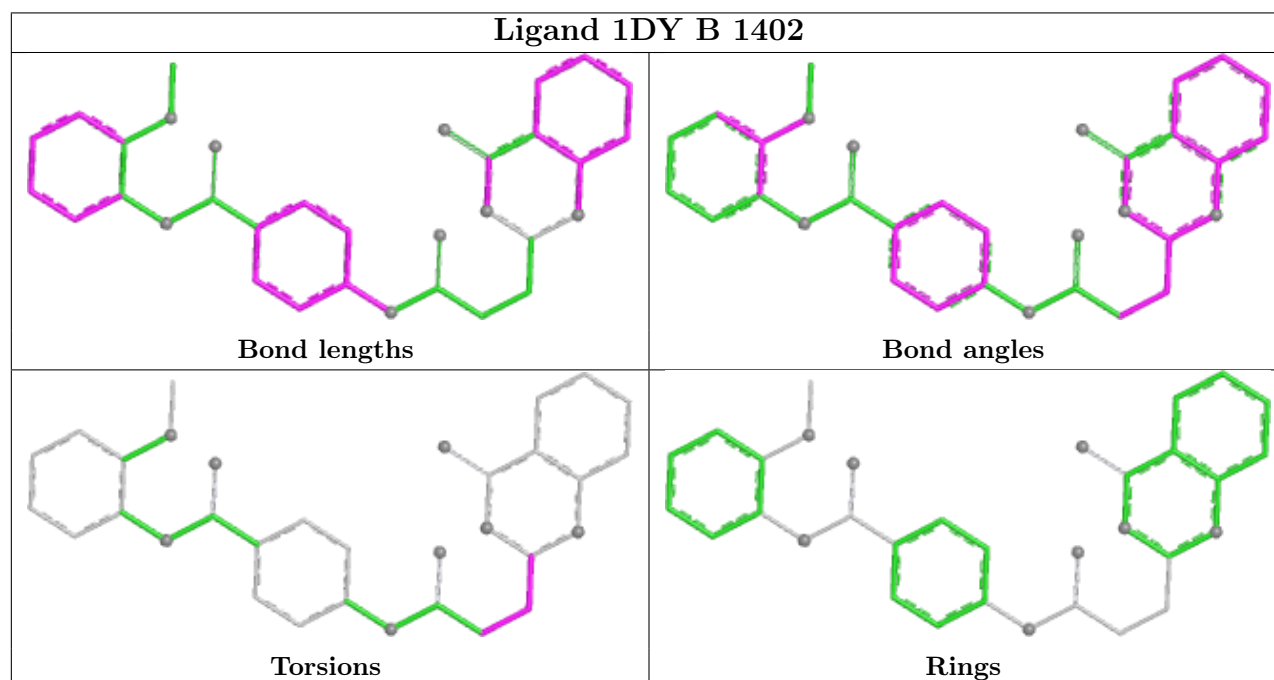
Mol	Chain	Res	Type	Atoms
3	A	1402	1DY	N1-C8-C9-C10
3	A	1402	1DY	N2-C8-C9-C10
3	B	1402	1DY	N1-C8-C9-C10
3	B	1402	1DY	N2-C8-C9-C10
3	A	1402	1DY	C11-C10-C9-C8
3	B	1402	1DY	C11-C10-C9-C8
3	C	1402	1DY	N1-C8-C9-C10
3	C	1402	1DY	N2-C8-C9-C10

There are no ring outliers.

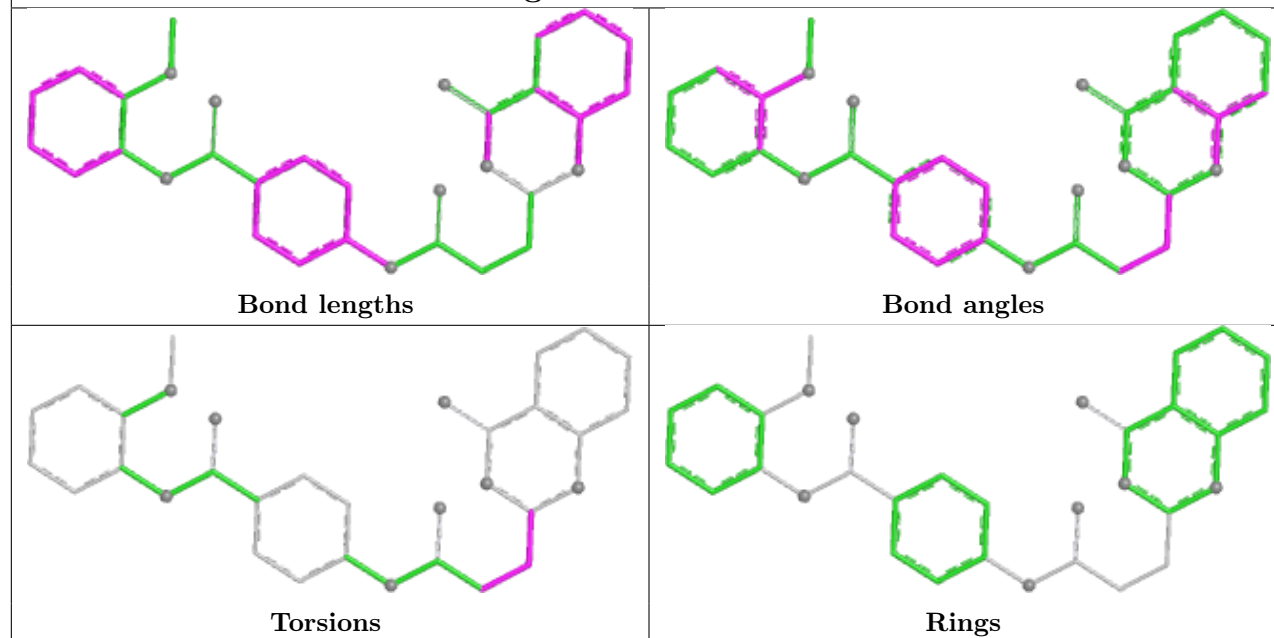
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1402	1DY	5	0
3	A	1402	1DY	3	0
3	D	1402	1DY	1	0
3	C	1402	1DY	2	0

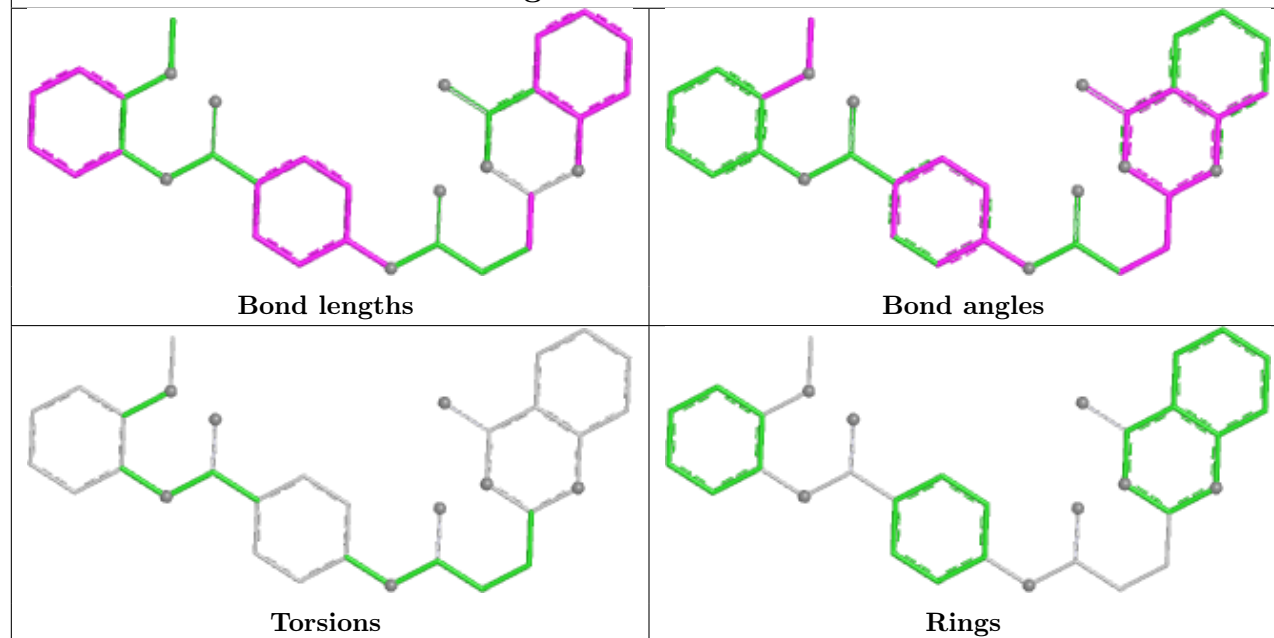
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

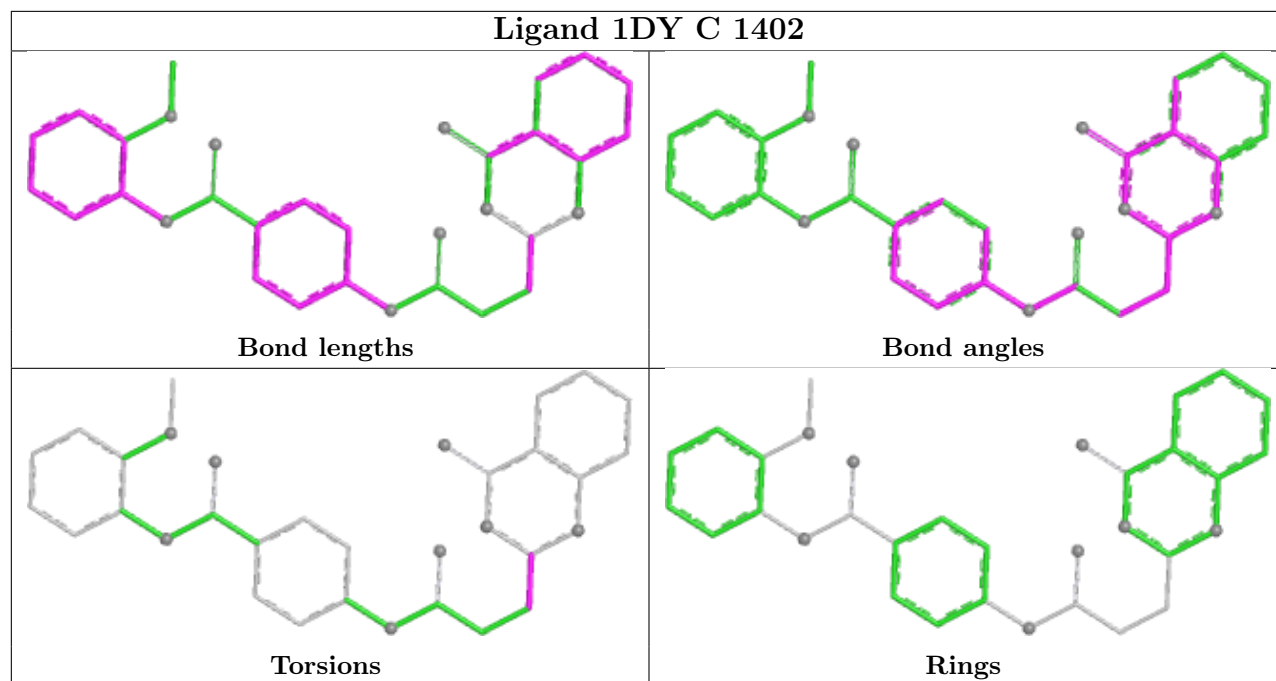


Ligand 1DY A 1402



Ligand 1DY D 1402





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	212/217 (97%)	0.50	15 (7%) 22 18	21, 37, 63, 82	0
1	B	211/217 (97%)	0.60	20 (9%) 14 11	19, 34, 67, 79	0
1	C	209/217 (96%)	0.71	22 (10%) 11 8	22, 38, 68, 73	0
1	D	206/217 (94%)	0.76	24 (11%) 9 7	22, 38, 67, 75	0
All	All	838/868 (96%)	0.64	81 (9%) 13 10	19, 37, 67, 82	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1203	TYR	5.2
1	B	1285	ASN	4.6
1	C	1230	GLY	4.5
1	D	1282	PRO	4.4
1	C	1285	ASN	4.3
1	B	1282	PRO	4.2
1	C	1228	ILE	4.2
1	D	1232	THR	4.2
1	D	1203	TYR	3.8
1	B	1283	SER	3.8
1	D	1137	ASN	3.7
1	D	1204	ILE	3.7
1	C	1229	GLY	3.6
1	D	1112	ALA	3.6
1	D	1228	ILE	3.6
1	C	1204	ILE	3.5
1	D	1138	ALA	3.5
1	D	1287	LEU	3.5
1	B	1281	ARG	3.3
1	A	1203	TYR	3.3
1	C	1283	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	1281	ARG	3.1
1	C	1284	VAL	3.1
1	A	1285	ASN	2.9
1	D	1230	GLY	2.9
1	B	1265	THR	2.9
1	B	1233	GLY	2.9
1	A	1104	GLN	2.8
1	D	1135	GLY	2.8
1	B	1204	ILE	2.8
1	D	1134	ASP	2.8
1	D	1144	ARG	2.8
1	A	1289	TYR	2.8
1	D	1312	LYS	2.8
1	A	1265	THR	2.7
1	B	1314	GLU	2.7
1	D	1205	GLY	2.7
1	B	1228	ILE	2.6
1	B	1284	VAL	2.6
1	A	1266	MET	2.6
1	A	1230	GLY	2.6
1	A	1315	HIS	2.6
1	D	1208	PHE	2.6
1	A	1228	ILE	2.5
1	B	1236	THR	2.5
1	C	1135	GLY	2.5
1	C	1232	THR	2.5
1	D	1234	CYS	2.5
1	C	1233	GLY	2.5
1	C	1287	LEU	2.4
1	A	1284	VAL	2.4
1	C	1134	ASP	2.4
1	B	1263	PHE	2.4
1	B	1262	GLN	2.4
1	A	1130	ARG	2.4
1	B	1132	HIS	2.4
1	D	1240	ARG	2.4
1	D	1265	THR	2.4
1	C	1202	ALA	2.4
1	B	1144	ARG	2.3
1	B	1289	TYR	2.3
1	C	1138	ALA	2.3
1	A	1171	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1235	PRO	2.2
1	D	1104	GLN	2.2
1	A	1313	PRO	2.2
1	C	1133	ARG	2.2
1	A	1263	PHE	2.2
1	D	1235	PRO	2.2
1	C	1282	PRO	2.2
1	B	1230	GLY	2.1
1	B	1287	LEU	2.1
1	B	1133	ARG	2.1
1	C	1171	GLU	2.1
1	C	1116	LYS	2.1
1	D	1229	GLY	2.1
1	D	1161	ARG	2.1
1	B	1104	GLN	2.1
1	D	1281	ARG	2.1
1	A	1236	THR	2.0
1	C	1207	MET	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, 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
3	1DY	D	1402	33/33	0.93	0.09	25,28,32,34	0
3	1DY	B	1402	33/33	0.95	0.08	21,25,29,30	0
3	1DY	C	1402	33/33	0.95	0.07	23,26,30,31	0
3	1DY	A	1402	33/33	0.95	0.08	24,26,30,33	0
2	ZN	D	1401	1/1	0.97	0.06	66,66,66,66	0

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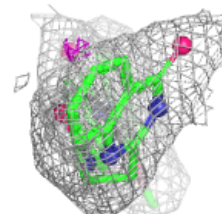
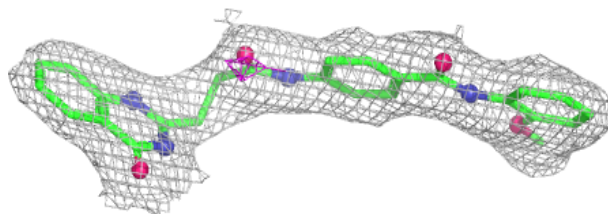
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	C	1401	1/1	0.98	0.04	59,59,59,59	0
2	ZN	B	1401	1/1	0.98	0.04	48,48,48,48	0
2	ZN	A	1401	1/1	0.99	0.02	52,52,52,52	0

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.

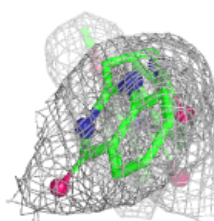
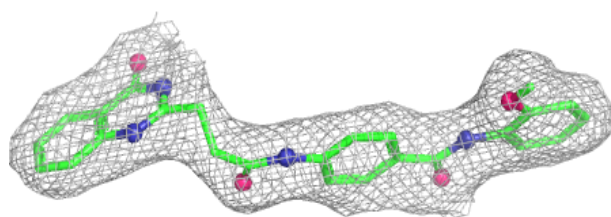
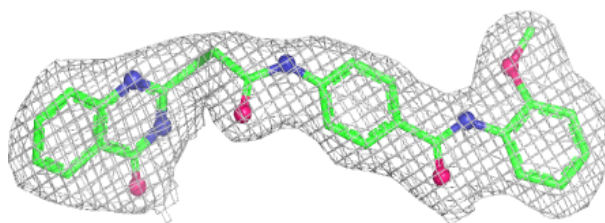
Electron density around 1DY D 1402:

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

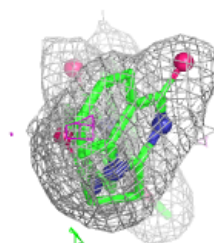
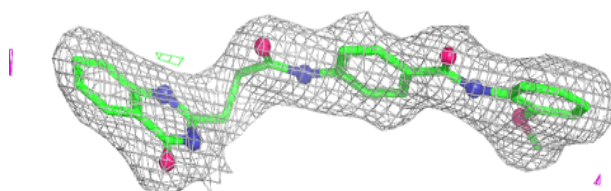
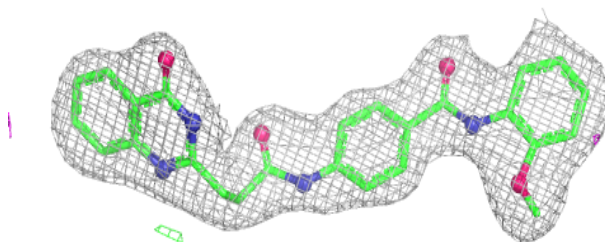


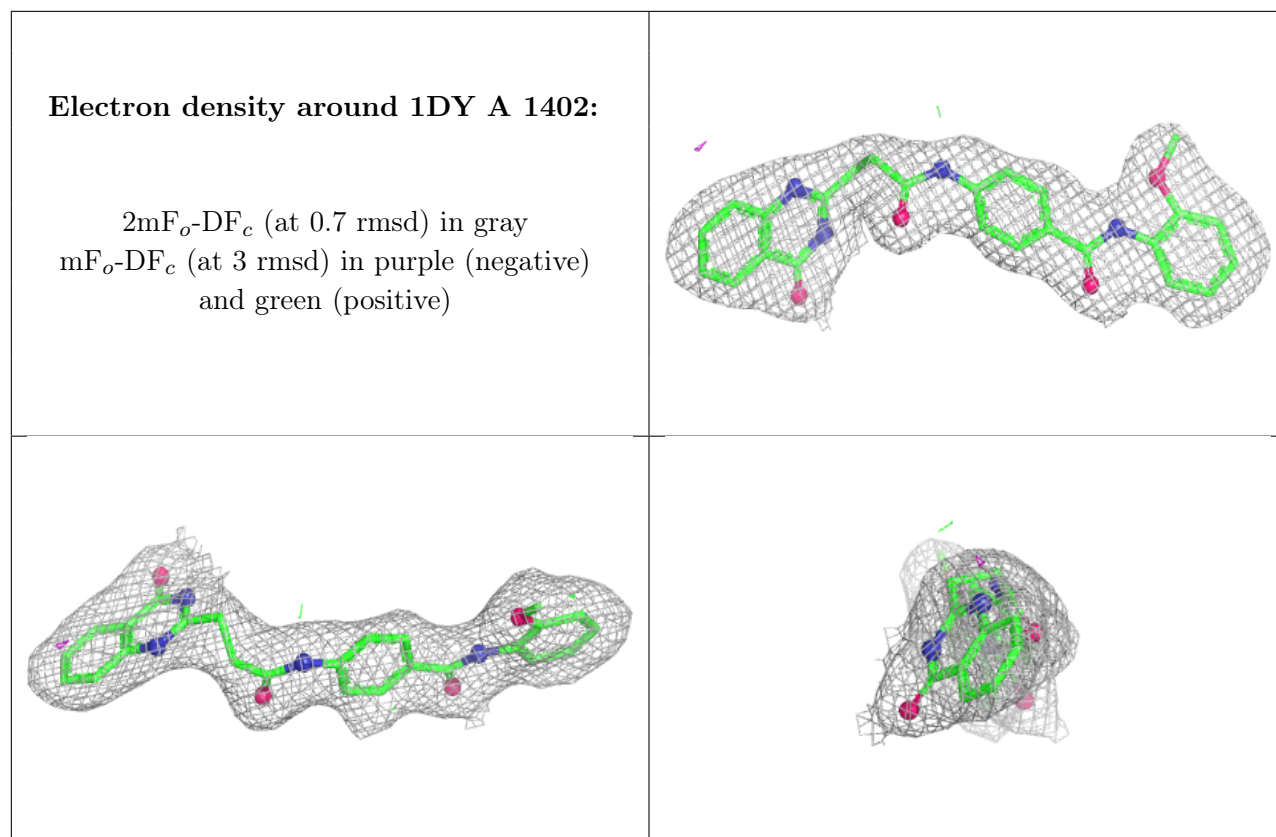
Electron density around 1DY B 1402:

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

**Electron density around 1DY C 1402:**

$2mF_o-DF_c$ (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.