



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:28 PM UTC

PDB ID : 2YX1 / pdb_00002yx1
Title : Crystal structure of M.jannaschii tRNA m1G37 methyltransferase
Authors : Goto-Ito, S.; Ito, T.; Ishii, R.; Bessho, Y.; Yokoyama, S.
Deposited on : 2007-04-23
Resolution : 2.20 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

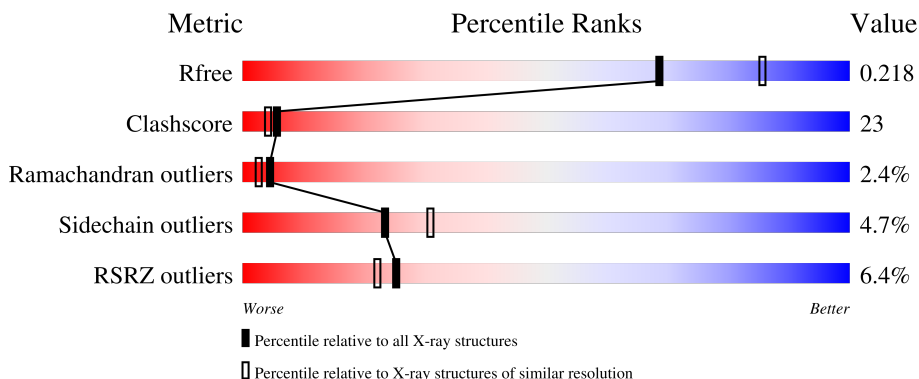
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	336	2% 60% 30% 6%
1	B	336	10% 58% 28% 5% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5485 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.

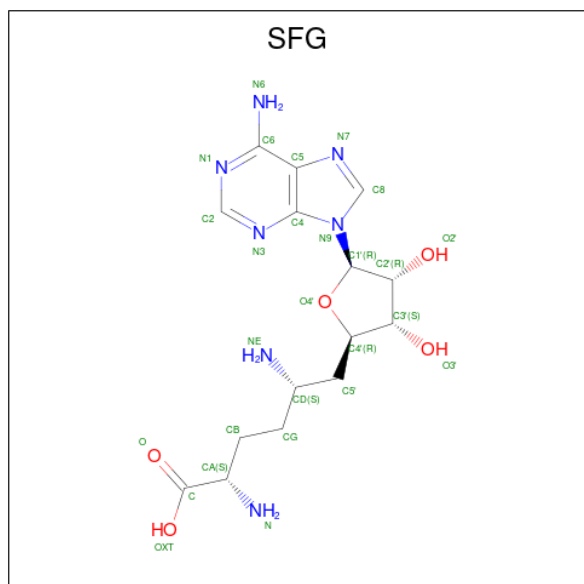
- Molecule 1 is a protein called Hypothetical protein MJ0883.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	Se	0	0	0
			2641	1704	453	476	5	3			
1	B	310	Total	C	N	O	S	Se	0	0	0
			2527	1634	431	454	5	3			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Zn	0	0
			4	4		
2	B	6	Total	Zn	0	0
			6	6		

- Molecule 3 is SINEFUNGIN (CCD ID: SFG) (formula: C₁₅H₂₃N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 27	C 15	N 7	O 5	0	0
3	B	1	Total 27	C 15	N 7	O 5	0	0

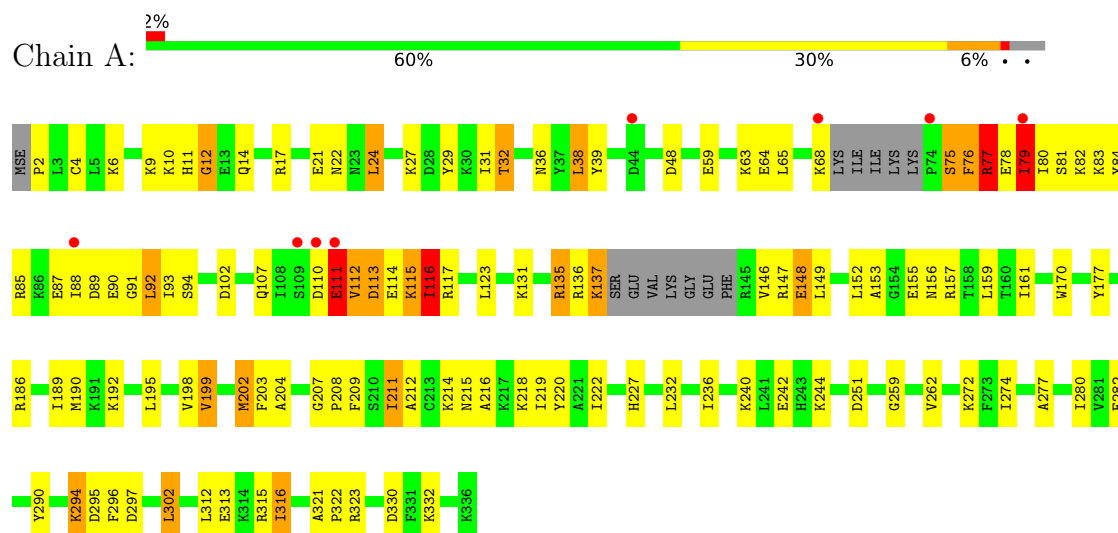
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total 149	O 149	0	0
4	B	104	Total 104	O 104	0	0

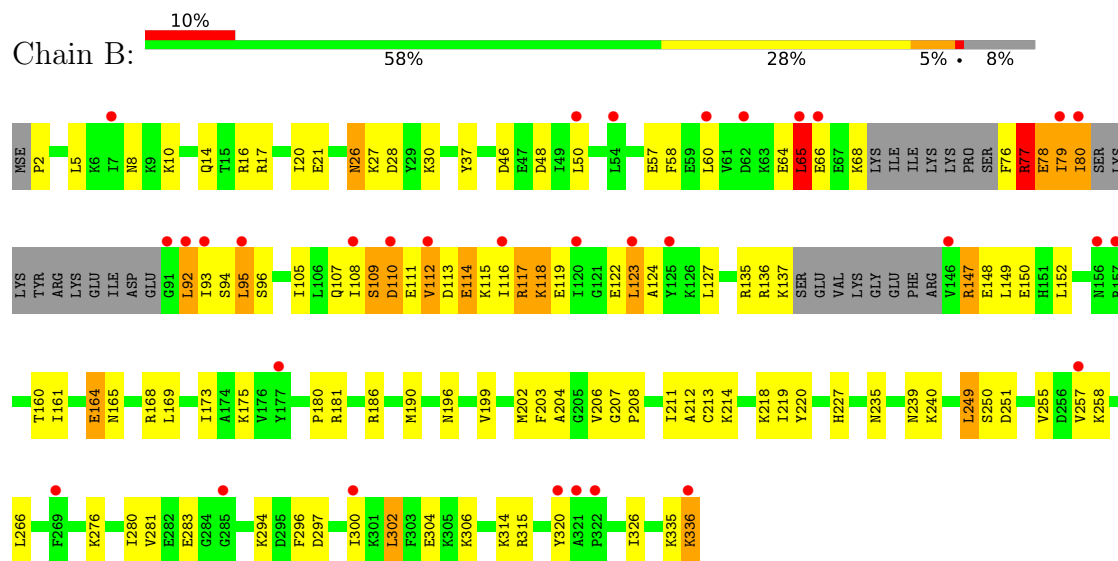
3 Residue-property plots

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: Hypothetical protein MJ0883



• Molecule 1: Hypothetical protein MJ0883



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.00Å 69.79Å 87.15Å 90.00° 96.07° 90.00°	Depositor
Resolution (Å)	47.90 – 2.20 47.90 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (47.90-2.20) 96.8 (47.90-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.224 , 0.276 0.227 , 0.218	Depositor DCC
R_{free} test set	1814 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5485	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% 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: SFG, 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	0.59	1/2678 (0.0%)	1.07	18/3581 (0.5%)
1	B	0.54	0/2561	1.04	13/3426 (0.4%)
All	All	0.57	1/5239 (0.0%)	1.05	31/7007 (0.4%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	VAL	CA-CB	5.41	1.61	1.54

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	LYS	N-CA-C	-10.36	100.43	112.87
1	B	66	GLU	N-CA-C	8.84	123.65	109.24
1	B	251	ASP	N-CA-C	-8.78	96.69	109.59
1	B	204	ALA	N-CA-C	8.75	121.97	111.82
1	A	204	ALA	N-CA-C	8.31	123.19	112.89
1	A	111	GLU	N-CA-C	-7.69	94.43	110.80
1	A	251	ASP	N-CA-C	-7.27	98.21	109.76
1	A	316	ILE	N-CA-C	-7.04	98.44	108.58
1	A	202	MSE	N-CA-C	6.92	118.82	111.28
1	B	117	ARG	N-CA-C	-6.47	97.02	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	95	LEU	N-CA-C	-6.46	105.22	113.23
1	B	297	ASP	N-CA-C	6.37	119.04	111.33
1	A	31	ILE	N-CA-C	-6.26	100.91	109.37
1	A	112	VAL	N-CA-C	-5.90	101.19	109.21
1	A	297	ASP	N-CA-C	5.87	118.15	111.11
1	B	124	ALA	N-CA-C	-5.72	105.12	111.36
1	A	79	ILE	N-CA-C	5.70	115.89	110.42
1	B	202	MSE	N-CA-C	5.63	117.42	111.28
1	A	77	ARG	N-CA-C	-5.61	105.17	111.28
1	A	294	LYS	N-CA-C	-5.60	106.45	113.28
1	B	294	LYS	N-CA-C	-5.58	105.58	112.90
1	A	135	ARG	N-CA-C	-5.56	100.67	108.96
1	A	198	VAL	N-CA-C	-5.52	99.69	107.75
1	B	199	VAL	N-CA-C	5.43	116.13	108.36
1	A	227	HIS	N-CA-C	-5.35	105.52	111.36
1	B	65	LEU	N-CA-C	5.22	121.91	110.80
1	A	296	PHE	N-CA-C	5.19	119.33	112.89
1	A	116	ILE	N-CA-C	-5.18	105.35	111.00
1	A	222	ILE	N-CA-C	5.16	116.01	108.53
1	B	180	PRO	N-CA-C	-5.08	107.52	113.86
1	A	211	ILE	N-CA-C	-5.03	105.64	110.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	37	TYR	Sidechain

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	2641	0	2779	131	0
1	B	2527	0	2659	119	1
2	A	4	0	0	0	0
2	B	6	0	0	0	0
3	A	27	0	21	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	21	0	0
4	A	149	0	0	10	2
4	B	104	0	0	2	0
All	All	5485	0	5480	251	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 23.

All (251) 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:202:MSE:HE1	1:A:277:ALA:HA	1.24	1.16
1:A:202:MSE:HE2	1:A:280:ILE:HD12	1.14	1.09
1:A:113:ASP:O	1:A:116:ILE:HG22	1.63	0.98
1:B:116:ILE:HG23	1:B:119:GLU:HG3	1.45	0.98
1:A:199:VAL:HB	1:A:219:ILE:HD12	1.47	0.93
1:A:216:ALA:HB3	1:A:219:ILE:HD11	1.51	0.92
1:A:202:MSE:HE3	1:A:262:VAL:HG11	1.51	0.92
1:A:4:CYS:SG	1:A:65:LEU:HD11	2.10	0.91
1:A:202:MSE:HE3	1:A:262:VAL:CG1	2.01	0.91
1:A:274:ILE:HB	4:A:610:HOH:O	1.73	0.87
1:A:202:MSE:HE1	1:A:277:ALA:CA	2.05	0.86
1:B:79:ILE:C	1:B:80:ILE:HD13	2.01	0.86
1:B:110:ASP:HA	1:B:135:ARG:HH12	1.41	0.86
1:A:80:ILE:HG22	1:A:88:ILE:HD11	1.58	0.84
1:B:116:ILE:HG23	1:B:119:GLU:CG	2.07	0.84
1:A:92:LEU:H	1:A:92:LEU:HD22	1.44	0.80
1:B:114:GLU:C	1:B:116:ILE:H	1.90	0.80
1:A:85:ARG:O	1:A:89:ASP:HB2	1.81	0.79
1:B:190:MSE:HE2	1:B:214:LYS:HE2	1.64	0.79
1:A:218:LYS:O	1:A:219:ILE:HD13	1.83	0.79
1:B:110:ASP:O	1:B:112:VAL:N	2.17	0.78
1:B:76:PHE:O	1:B:79:ILE:HG12	1.84	0.77
1:B:17:ARG:O	1:B:21:GLU:HG3	1.85	0.77
1:B:135:ARG:HB2	1:B:152:LEU:HD11	1.69	0.75
1:B:276:LYS:NZ	1:B:280:ILE:HD11	2.02	0.74
1:A:202:MSE:CE	1:A:277:ALA:HA	2.13	0.73
1:B:169:LEU:CD2	1:B:211:ILE:HD12	2.19	0.73
1:B:137:LYS:HD2	1:B:148:GLU:HG3	1.69	0.72
1:A:22:ASN:HD22	1:A:316:ILE:H	1.36	0.71
1:B:8:ASN:HD22	1:B:10:LYS:H	1.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:HG3	1:A:115:LYS:N	2.04	0.70
1:A:22:ASN:O	1:A:24:LEU:HD13	1.93	0.69
1:B:276:LYS:HZ2	1:B:280:ILE:HD11	1.54	0.69
1:B:181:ARG:HH11	1:B:181:ARG:HG3	1.58	0.68
1:B:114:GLU:HG2	1:B:115:LYS:N	2.09	0.68
1:A:274:ILE:HD12	1:A:302:LEU:HD22	1.77	0.67
1:A:91:GLY:O	1:A:93:ILE:N	2.28	0.66
1:A:110:ASP:O	1:A:111:GLU:HG3	1.96	0.66
1:B:117:ARG:C	1:B:119:GLU:H	2.04	0.66
1:A:115:LYS:HE2	1:A:115:LYS:HA	1.76	0.66
1:B:116:ILE:HG12	1:B:119:GLU:OE1	1.96	0.66
1:B:92:LEU:O	1:B:93:ILE:HG12	1.97	0.65
1:B:21:GLU:O	1:B:315:ARG:HD3	1.95	0.65
1:A:202:MSE:CE	1:A:262:VAL:HG11	2.25	0.65
1:B:117:ARG:C	1:B:119:GLU:N	2.50	0.65
1:B:78:GLU:CD	1:B:78:GLU:H	2.05	0.65
1:B:211:ILE:HD11	1:B:235:ASN:HB3	1.78	0.64
1:A:75:SER:HB3	1:A:78:GLU:CB	2.28	0.64
1:A:94:SER:HB3	1:A:107:GLN:HB3	1.78	0.64
1:B:2:PRO:HD2	1:B:65:LEU:HG	1.79	0.64
1:A:135:ARG:HG2	1:A:152:LEU:HD11	1.80	0.64
1:A:148:GLU:CD	1:A:148:GLU:H	2.06	0.64
1:B:116:ILE:O	1:B:116:ILE:HG22	1.96	0.63
1:B:16:ARG:NH1	1:B:20:ILE:HD11	2.14	0.63
1:A:116:ILE:HD13	1:A:116:ILE:O	1.98	0.63
1:B:93:ILE:HD11	1:B:108:ILE:HG23	1.79	0.62
1:B:93:ILE:HD13	1:B:108:ILE:HA	1.80	0.62
1:A:90:GLU:HG3	1:A:92:LEU:HD23	1.81	0.62
1:A:113:ASP:C	1:A:116:ILE:HG22	2.24	0.62
1:A:81:SER:O	1:A:85:ARG:HB2	1.99	0.62
1:A:27:LYS:O	1:A:68:LYS:HD2	2.00	0.61
1:A:75:SER:HB3	1:A:78:GLU:HB3	1.82	0.61
1:A:110:ASP:CG	1:A:135:ARG:HH12	2.07	0.61
1:A:131:LYS:O	1:A:155:GLU:N	2.34	0.61
1:B:92:LEU:HB2	1:B:109:SER:HB2	1.83	0.61
1:A:159:LEU:HD11	1:A:170:TRP:CE3	2.35	0.60
1:B:147:ARG:HB2	1:B:147:ARG:HH21	1.67	0.59
1:A:312:LEU:HD11	1:A:332:LYS:HB2	1.84	0.59
1:A:321:ALA:HB1	1:A:322:PRO:HD2	1.83	0.59
1:A:190:MSE:HE3	1:A:212:ALA:HA	1.85	0.59
1:A:186:ARG:NH2	4:A:537:HOH:O	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:MSE:HE3	1:A:262:VAL:HG13	1.86	0.58
1:A:79:ILE:HG12	1:A:123:LEU:HD21	1.86	0.58
1:A:152:LEU:O	1:A:153:ALA:HB2	2.02	0.58
1:A:232:LEU:O	1:A:236:ILE:HG13	2.04	0.58
1:B:92:LEU:HD22	1:B:109:SER:OG	2.03	0.58
1:A:75:SER:OG	1:A:77:ARG:HG2	2.04	0.58
1:B:16:ARG:NH1	1:B:20:ILE:CD1	2.67	0.57
1:A:159:LEU:HD11	1:A:170:TRP:CZ3	2.40	0.57
1:B:137:LYS:HD2	1:B:148:GLU:CG	2.35	0.57
1:A:64:GLU:O	1:A:65:LEU:HD23	2.03	0.57
1:B:108:ILE:O	1:B:109:SER:C	2.47	0.56
1:B:168:ARG:H	1:B:239:ASN:HD21	1.51	0.56
1:A:48:ASP:OD2	1:A:323:ARG:NH2	2.39	0.56
1:B:320:TYR:HB2	1:B:326:ILE:HD12	1.86	0.56
1:A:244:LYS:HD2	4:A:593:HOH:O	2.04	0.56
1:B:137:LYS:HB2	1:B:148:GLU:HG3	1.87	0.56
1:A:202:MSE:CE	1:A:280:ILE:HD12	2.09	0.55
1:B:76:PHE:O	1:B:78:GLU:N	2.39	0.55
1:A:14:GLN:NE2	1:A:17:ARG:HH21	2.04	0.55
1:B:110:ASP:CA	1:B:135:ARG:HH12	2.17	0.55
1:B:78:GLU:C	1:B:80:ILE:H	2.13	0.55
1:A:190:MSE:CE	1:A:214:LYS:HE3	2.37	0.55
1:B:26:ASN:C	1:B:26:ASN:HD22	2.14	0.55
1:A:92:LEU:HD12	1:A:111:GLU:HB2	1.89	0.55
1:B:76:PHE:CD1	1:B:79:ILE:HD11	2.42	0.55
1:B:190:MSE:CE	1:B:214:LYS:HE2	2.37	0.55
1:B:92:LEU:HD22	1:B:109:SER:CB	2.38	0.54
1:A:195:LEU:HD13	4:A:609:HOH:O	2.06	0.54
1:A:199:VAL:CB	1:A:219:ILE:HD12	2.30	0.54
1:B:116:ILE:CG2	1:B:119:GLU:HG3	2.28	0.54
1:B:169:LEU:HD23	1:B:211:ILE:HD12	1.88	0.54
1:B:118:LYS:O	1:B:122:GLU:HG2	2.06	0.54
1:A:148:GLU:OE1	1:A:148:GLU:N	2.41	0.54
1:A:2:PRO:HG2	1:A:29:TYR:CE2	2.44	0.53
1:B:326:ILE:HD12	1:B:326:ILE:N	2.23	0.53
1:A:79:ILE:HG13	1:A:80:ILE:N	2.23	0.53
1:A:137:LYS:CB	1:A:147:ARG:HH11	2.21	0.53
1:B:76:PHE:O	1:B:77:ARG:C	2.51	0.53
1:B:110:ASP:OD1	1:B:137:LYS:C	2.52	0.53
1:B:135:ARG:HB2	1:B:152:LEU:CD1	2.38	0.53
1:A:218:LYS:C	1:A:219:ILE:HD13	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:OD2	1:A:157:ARG:NH2	2.42	0.52
1:B:93:ILE:CD1	1:B:108:ILE:HG23	2.39	0.52
1:B:320:TYR:HB2	1:B:326:ILE:CD1	2.40	0.52
1:B:27:LYS:O	1:B:68:LYS:NZ	2.42	0.52
1:B:116:ILE:HG23	1:B:119:GLU:CD	2.34	0.52
1:A:85:ARG:O	1:A:89:ASP:CB	2.54	0.52
1:A:102:ASP:OD1	1:A:131:LYS:HB2	2.10	0.52
1:B:105:ILE:HD12	1:B:105:ILE:N	2.25	0.52
1:B:136:ARG:HD2	1:B:147:ARG:HB3	1.90	0.52
1:B:296:PHE:CD2	1:B:314:LYS:HD2	2.45	0.52
1:A:32:THR:CG2	1:A:65:LEU:HD22	2.39	0.52
1:B:186:ARG:NH2	4:B:519:HOH:O	2.42	0.51
1:B:80:ILE:HD13	1:B:80:ILE:N	2.25	0.51
1:B:114:GLU:C	1:B:116:ILE:N	2.58	0.51
1:A:84:TYR:CE1	1:A:116:ILE:HD11	2.46	0.51
1:B:14:GLN:NE2	1:B:17:ARG:HE	2.08	0.51
1:A:77:ARG:O	1:A:81:SER:HB2	2.11	0.51
1:B:30:LYS:HG2	1:B:68:LYS:HD2	1.92	0.51
1:B:123:LEU:HD11	1:B:127:LEU:HD12	1.93	0.50
1:B:190:MSE:HE3	1:B:212:ALA:HA	1.93	0.50
1:A:218:LYS:NZ	4:A:648:HOH:O	2.45	0.50
1:B:213:CYS:O	1:B:219:ILE:HD11	2.12	0.50
1:A:161:ILE:HD11	1:A:170:TRP:CZ2	2.45	0.50
1:A:207:GLY:N	1:A:208:PRO:HD3	2.26	0.50
1:A:79:ILE:HD11	1:A:83:LYS:HE2	1.92	0.50
1:B:114:GLU:HG2	1:B:115:LYS:H	1.75	0.50
1:B:26:ASN:ND2	1:B:28:ASP:H	2.10	0.49
1:B:255:VAL:HG12	1:B:257:VAL:HG23	1.94	0.49
1:A:137:LYS:HB2	1:A:147:ARG:HH11	1.78	0.49
1:B:14:GLN:HE21	1:B:17:ARG:HE	1.60	0.49
1:A:32:THR:HG21	1:A:65:LEU:HD22	1.94	0.49
1:B:96:SER:HB2	1:B:181:ARG:HH21	1.78	0.49
1:B:336:LYS:HD2	4:B:536:HOH:O	2.12	0.49
1:A:75:SER:CB	1:A:78:GLU:HB2	2.43	0.48
1:B:302:LEU:HD21	1:B:306:LYS:HZ3	1.77	0.48
1:A:88:ILE:HG12	1:A:93:ILE:HB	1.96	0.48
1:A:159:LEU:C	1:A:159:LEU:HD13	2.38	0.48
1:B:5:LEU:HD11	1:B:58:PHE:HB2	1.96	0.48
1:B:150:GLU:OE1	1:B:152:LEU:HD21	2.14	0.48
1:B:109:SER:O	1:B:110:ASP:O	2.32	0.48
1:B:181:ARG:HG3	1:B:181:ARG:NH1	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:LEU:O	1:B:250:SER:HB2	2.14	0.48
1:A:75:SER:HB3	1:A:78:GLU:HB2	1.94	0.48
1:A:156:ASN:O	1:A:156:ASN:ND2	2.47	0.48
1:B:164:GLU:OE1	1:B:186:ARG:HD2	2.12	0.48
1:A:92:LEU:HD22	1:A:92:LEU:N	2.22	0.48
1:A:207:GLY:O	1:A:211:ILE:HG12	2.14	0.47
1:A:189:ILE:HD11	1:A:290:TYR:OH	2.13	0.47
1:B:14:GLN:NE2	1:B:17:ARG:HH21	2.13	0.47
1:B:283:GLU:OE2	1:B:335:LYS:HD2	2.14	0.47
1:A:177:TYR:CE2	4:A:626:HOH:O	2.67	0.47
1:A:75:SER:O	1:A:76:PHE:CB	2.61	0.47
1:A:110:ASP:HB3	1:A:135:ARG:NH1	2.29	0.47
1:A:148:GLU:CD	1:A:148:GLU:N	2.72	0.46
1:B:77:ARG:HH11	1:B:95:LEU:HB3	1.80	0.46
1:A:136:ARG:NH2	4:A:621:HOH:O	2.48	0.46
1:A:113:ASP:O	1:A:117:ARG:HD3	2.15	0.46
1:A:177:TYR:HE1	4:A:627:HOH:O	1.97	0.46
1:A:189:ILE:HD12	1:A:209:PHE:HE2	1.81	0.46
1:A:10:LYS:HE3	1:A:11:HIS:NE2	2.31	0.46
1:A:22:ASN:ND2	1:A:316:ILE:H	2.08	0.46
1:B:50:LEU:HD12	1:B:60:LEU:HD11	1.98	0.46
1:B:220:TYR:CD2	1:B:257:VAL:HG11	2.51	0.45
1:A:85:ARG:HG3	1:A:85:ARG:HH11	1.81	0.45
1:B:149:LEU:HD11	1:B:173:ILE:HG13	1.97	0.45
1:B:76:PHE:CD1	1:B:123:LEU:HD12	2.51	0.45
1:B:218:LYS:C	1:B:219:ILE:HG13	2.41	0.45
1:A:202:MSE:HE1	1:A:277:ALA:CB	2.46	0.45
1:B:109:SER:C	1:B:110:ASP:O	2.58	0.45
1:A:259:GLY:O	1:A:282:GLU:HG3	2.16	0.45
1:A:294:LYS:HG3	1:A:295:ASP:OD2	2.17	0.45
1:B:76:PHE:HD1	1:B:123:LEU:CD1	2.29	0.45
1:A:91:GLY:O	1:A:92:LEU:C	2.59	0.45
1:A:110:ASP:CG	1:A:135:ARG:NH1	2.74	0.45
1:B:8:ASN:ND2	1:B:10:LYS:H	2.12	0.45
1:A:137:LYS:HB3	1:A:137:LYS:HE3	1.77	0.44
1:B:76:PHE:CE1	1:B:79:ILE:HD11	2.52	0.44
1:A:77:ARG:NH1	1:A:77:ARG:HG3	2.33	0.44
1:B:80:ILE:HG12	1:B:80:ILE:O	2.16	0.44
1:B:92:LEU:O	1:B:93:ILE:CG1	2.65	0.44
1:B:93:ILE:CD1	1:B:108:ILE:HA	2.47	0.44
1:A:114:GLU:HG3	1:A:115:LYS:H	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:HG2	1:A:149:LEU:CD2	2.48	0.44
1:B:206:VAL:CG2	1:B:208:PRO:HD3	2.47	0.44
1:A:17:ARG:O	1:A:21:GLU:HG2	2.18	0.44
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.83	0.43
1:B:26:ASN:C	1:B:26:ASN:ND2	2.76	0.43
1:B:26:ASN:HD22	1:B:27:LYS:N	2.16	0.43
1:A:218:LYS:HE3	1:A:220:TYR:CZ	2.53	0.43
1:B:94:SER:HB3	1:B:107:GLN:HB2	2.00	0.43
1:A:102:ASP:CG	1:A:157:ARG:HH22	2.26	0.43
1:B:164:GLU:HG3	1:B:165:ASN:ND2	2.34	0.43
1:B:203:PHE:CE1	1:B:266:LEU:HD22	2.53	0.43
1:A:12:GLY:HA2	1:A:38:LEU:HD12	2.00	0.43
1:A:116:ILE:HD13	1:A:116:ILE:C	2.43	0.43
1:B:113:ASP:O	1:B:114:GLU:CB	2.66	0.43
1:B:115:LYS:O	1:B:118:LYS:HG3	2.19	0.43
1:B:257:VAL:HG12	1:B:258:LYS:N	2.34	0.43
1:B:300:ILE:O	1:B:304:GLU:HG3	2.18	0.43
1:A:2:PRO:N	1:A:63:LYS:O	2.51	0.42
1:A:9:LYS:HE2	1:A:36:ASN:HA	2.01	0.42
1:A:10:LYS:CE	4:A:604:HOH:O	2.67	0.42
1:A:112:VAL:HG23	1:A:117:ARG:CD	2.49	0.42
1:B:276:LYS:O	1:B:280:ILE:HG12	2.20	0.42
1:B:95:LEU:HD12	1:B:95:LEU:N	2.35	0.42
1:B:113:ASP:O	1:B:114:GLU:HB2	2.20	0.42
1:A:192:LYS:HE2	1:A:330:ASP:OD2	2.20	0.42
1:A:192:LYS:NZ	1:A:313:GLU:OE1	2.41	0.42
3:A:401:SFG:HG2	3:A:401:SFG:H4'	1.91	0.42
1:B:175:LYS:HE2	1:B:227:HIS:ND1	2.33	0.42
1:A:136:ARG:C	1:A:137:LYS:HD2	2.45	0.42
1:A:82:LYS:HG3	1:A:83:LYS:N	2.34	0.42
1:A:218:LYS:HE3	1:A:220:TYR:OH	2.20	0.42
1:B:207:GLY:N	1:B:208:PRO:HD3	2.35	0.42
1:B:46:ASP:OD1	1:B:48:ASP:HB2	2.20	0.42
1:A:79:ILE:O	1:A:82:LYS:HG2	2.20	0.41
1:A:75:SER:O	1:A:76:PHE:HB2	2.20	0.41
1:B:78:GLU:O	1:B:79:ILE:HB	2.20	0.41
1:B:115:LYS:HE2	1:B:118:LYS:NZ	2.35	0.41
1:B:281:VAL:O	1:B:336:LYS:HE2	2.20	0.41
1:A:161:ILE:HD11	1:A:170:TRP:CE2	2.54	0.41
1:A:21:GLU:HB2	1:A:315:ARG:CZ	2.50	0.41
1:A:137:LYS:HB3	1:A:147:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLU:HB3	1:A:92:LEU:HB2	2.02	0.41
1:A:136:ARG:HG2	1:A:149:LEU:HD23	2.02	0.41
1:A:272:LYS:HD3	4:A:568:HOH:O	2.21	0.41
1:B:160:THR:OG1	1:B:161:ILE:N	2.53	0.41
1:B:78:GLU:C	1:B:80:ILE:N	2.79	0.41
1:A:203:PHE:HB3	3:A:401:SFG:O4'	2.20	0.41
1:B:92:LEU:HD22	1:B:109:SER:HB2	2.02	0.41
1:B:127:LEU:HA	1:B:127:LEU:HD23	1.80	0.41
1:A:79:ILE:O	1:A:79:ILE:HD12	2.21	0.40
1:B:79:ILE:C	1:B:80:ILE:CD1	2.84	0.40
1:A:79:ILE:HD12	1:A:79:ILE:C	2.46	0.40
1:A:112:VAL:HG23	1:A:117:ARG:HD3	2.04	0.40
1:A:207:GLY:N	1:A:208:PRO:CD	2.85	0.40
1:A:146:VAL:O	1:A:146:VAL:HG13	2.21	0.40
1:A:216:ALA:HB3	1:A:219:ILE:CD1	2.38	0.40
1:A:6:LYS:HE3	1:A:39:TYR:OH	2.21	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)
4:A:507:HOH:O	4:A:625:HOH:O[2_755]	2.07	0.13
1:B:64:GLU:OE2	4:A:604:HOH:O[2_746]	2.13	0.07

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	317/336 (94%)	287 (90%)	24 (8%)	6 (2%)	6	4
1	B	302/336 (90%)	271 (90%)	22 (7%)	9 (3%)	3	1
All	All	619/672 (92%)	558 (90%)	46 (7%)	15 (2%)	4	3

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	PHE
1	A	92	LEU
1	A	111	GLU
1	B	77	ARG
1	B	79	ILE
1	B	111	GLU
1	B	114	GLU
1	A	75	SER
1	B	78	GLU
1	B	110	ASP
1	A	113	ASP
1	B	92	LEU
1	B	109	SER
1	A	12	GLY
1	B	112	VAL

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	293/301 (97%)	279 (95%)	14 (5%)	23	30
1	B	280/301 (93%)	267 (95%)	13 (5%)	24	32
All	All	573/602 (95%)	546 (95%)	27 (5%)	23	31

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	32	THR
1	A	38	LEU
1	A	59	GLU
1	A	77	ARG
1	A	79	ILE
1	A	115	LYS
1	A	116	ILE

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Mol	Chain	Res	Type
1	A	137	LYS
1	A	148	GLU
1	A	215	ASN
1	A	240	LYS
1	A	242	GLU
1	A	302	LEU
1	B	26	ASN
1	B	57	GLU
1	B	65	LEU
1	B	77	ARG
1	B	80	ILE
1	B	123	LEU
1	B	147	ARG
1	B	164	GLU
1	B	196	ASN
1	B	240	LYS
1	B	249	LEU
1	B	302	LEU
1	B	336	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	22	ASN
1	A	151	HIS
1	A	156	ASN
1	A	215	ASN
1	B	8	ASN
1	B	14	GLN
1	B	26	ASN
1	B	107	GLN
1	B	151	HIS
1	B	156	ASN
1	B	239	ASN
1	B	334	ASN

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 10 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$
3	SFG	A	401	2	28,29,29	1.00	3 (10%)	34,42,42	1.98	10 (29%)
3	SFG	B	402	2	28,29,29	1.01	3 (10%)	34,42,42	1.95	10 (29%)

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	SFG	A	401	2	-	0/17/33/33	0/3/3/3
3	SFG	B	402	2	-	0/17/33/33	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	SFG	C5-N7	-3.12	1.33	1.39
3	A	401	SFG	C5-N7	-3.07	1.33	1.39
3	B	402	SFG	C8-N9	-2.32	1.33	1.37
3	A	401	SFG	C8-N9	-2.32	1.33	1.37
3	A	401	SFG	C4-N9	-2.06	1.33	1.37
3	B	402	SFG	C4-N9	-2.06	1.33	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	SFG	C5-C4-N3	-5.24	119.50	126.72
3	B	402	SFG	C5-C4-N3	-5.21	119.54	126.72
3	A	401	SFG	N3-C2-N1	-4.70	121.47	128.58
3	B	402	SFG	N3-C2-N1	-4.64	121.56	128.58
3	A	401	SFG	N3-C4-N9	3.72	133.50	127.17
3	B	402	SFG	N3-C4-N9	3.65	133.38	127.17
3	A	401	SFG	C2-N3-C4	3.62	120.68	111.83
3	B	402	SFG	C2-N3-C4	3.59	120.60	111.83
3	A	401	SFG	N9-C8-N7	-3.20	109.39	113.94
3	B	402	SFG	N9-C8-N7	-3.15	109.47	113.94
3	B	402	SFG	C5-N7-C8	2.89	107.99	103.45
3	A	401	SFG	C5-N7-C8	2.89	107.99	103.45
3	B	402	SFG	C4-C5-N7	-2.85	107.33	110.58
3	A	401	SFG	C4-C5-N7	-2.81	107.36	110.58
3	A	401	SFG	C4'-O4'-C1'	-2.51	103.92	109.47
3	A	401	SFG	C4-N9-C8	2.40	108.25	105.74
3	B	402	SFG	O4'-C1'-C2'	-2.37	101.54	106.62
3	A	401	SFG	O4'-C1'-C2'	-2.33	101.63	106.62
3	B	402	SFG	C4-N9-C8	2.27	108.12	105.74
3	B	402	SFG	C4'-O4'-C1'	-2.14	104.73	109.47

There are no chirality outliers.

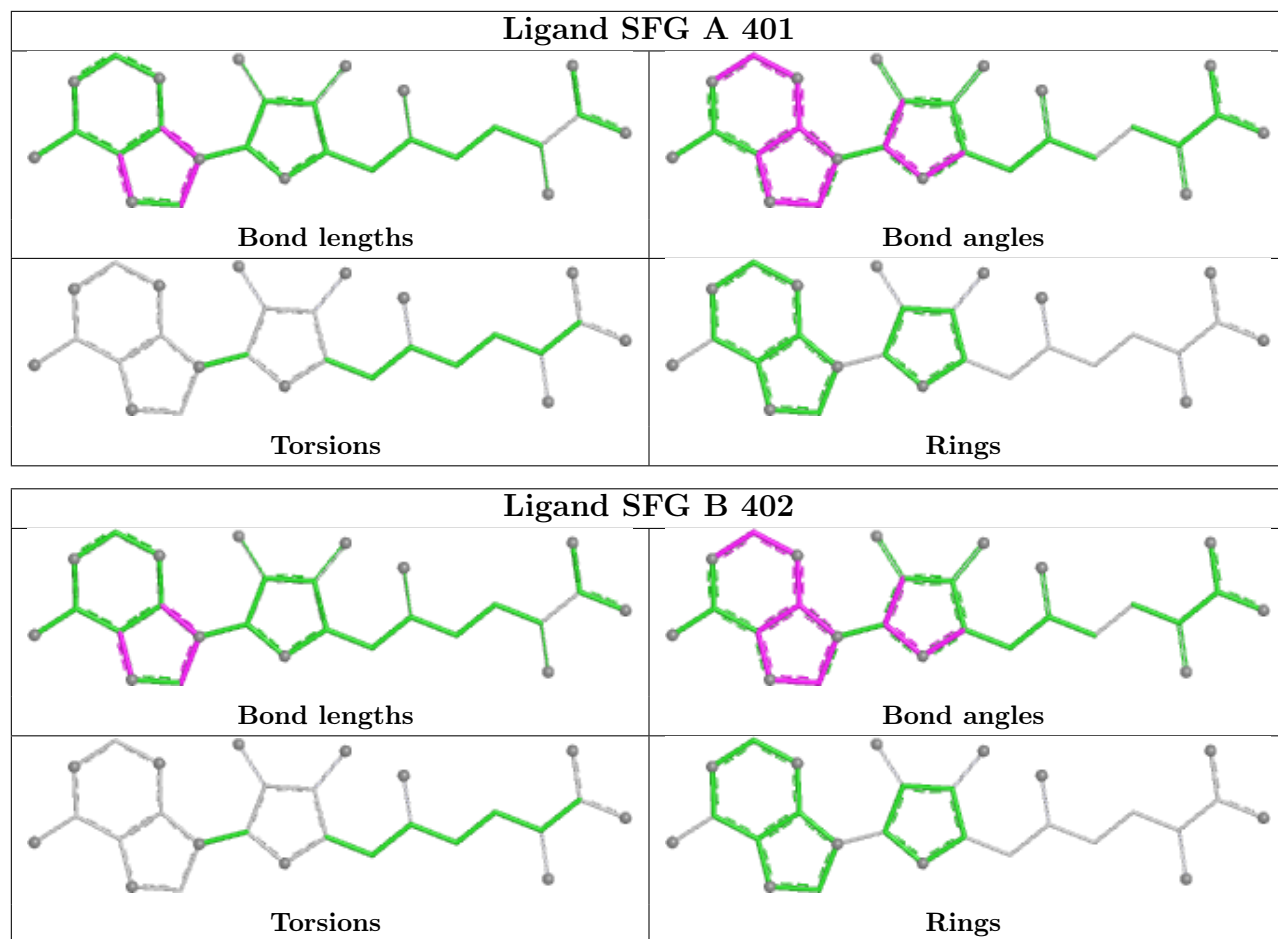
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SFG	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

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	320/336 (95%)	0.16	8 (2%) 58 55	18, 39, 82, 100	0
1	B	307/336 (91%)	1.03	32 (10%) 11 9	25, 44, 85, 108	0
All	All	627/672 (93%)	0.58	40 (6%) 25 22	18, 41, 84, 108	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	GLY	5.8
1	A	74	PRO	4.6
1	B	80	ILE	4.1
1	B	95	LEU	3.6
1	B	92	LEU	3.5
1	B	257	VAL	3.3
1	B	79	ILE	3.2
1	B	112	VAL	3.0
1	B	146	VAL	2.9
1	B	66	GLU	2.9
1	B	322	PRO	2.9
1	B	336	LYS	2.9
1	B	320	TYR	2.8
1	B	62	ASP	2.8
1	B	177	TYR	2.8
1	B	116	ILE	2.7
1	B	120	ILE	2.6
1	A	109	SER	2.6
1	A	44	ASP	2.6
1	B	110	ASP	2.5
1	A	111	GLU	2.4
1	B	60	LEU	2.4
1	B	321	ALA	2.4
1	B	300	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	285	GLY	2.4
1	A	88	ILE	2.4
1	B	125	TYR	2.3
1	B	54	LEU	2.3
1	B	157	ARG	2.3
1	B	156	ASN	2.2
1	B	65	LEU	2.2
1	A	79	ILE	2.1
1	B	269	PHE	2.1
1	A	110	ASP	2.1
1	B	123	LEU	2.1
1	B	93	ILE	2.1
1	B	50	LEU	2.0
1	B	7	ILE	2.0
1	B	108	ILE	2.0
1	A	68	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	B	509	1/1	0.82	0.14	80,80,80,80	0
2	ZN	B	505	1/1	0.87	0.10	39,39,39,39	0
2	ZN	B	508	1/1	0.89	0.11	67,67,67,67	0
2	ZN	B	510	1/1	0.90	0.10	71,71,71,71	0
3	SFG	B	402	27/27	0.91	0.09	19,30,36,41	0
3	SFG	A	401	27/27	0.95	0.07	19,25,36,41	0
2	ZN	B	506	1/1	0.95	0.06	47,47,47,47	0

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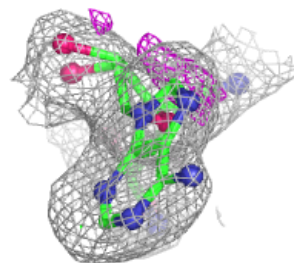
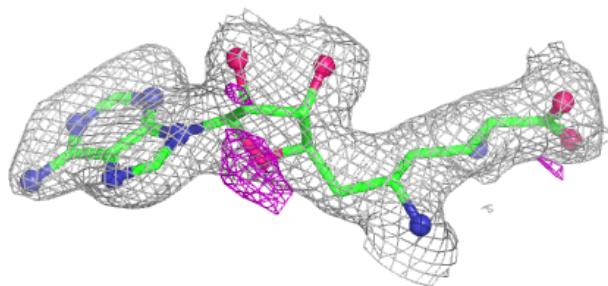
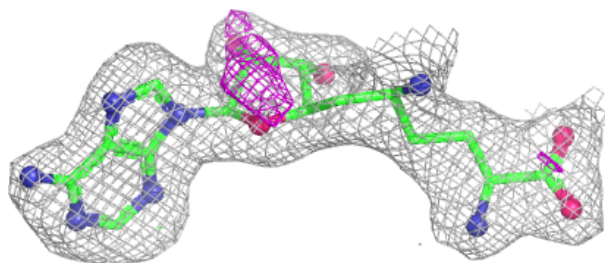
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	B	507	1/1	0.96	0.08	70,70,70,70	0
2	ZN	A	503	1/1	0.97	0.07	77,77,77,77	0
2	ZN	A	504	1/1	0.98	0.04	53,53,53,53	0
2	ZN	A	501	1/1	0.99	0.03	33,33,33,33	0
2	ZN	A	502	1/1	0.99	0.03	31,31,31,31	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.

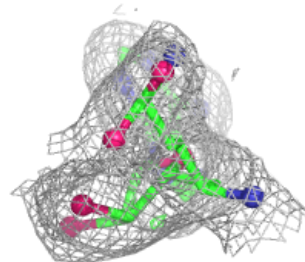
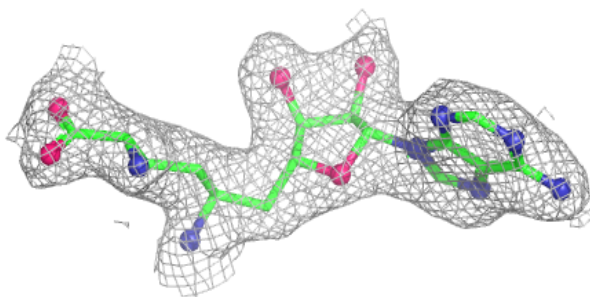
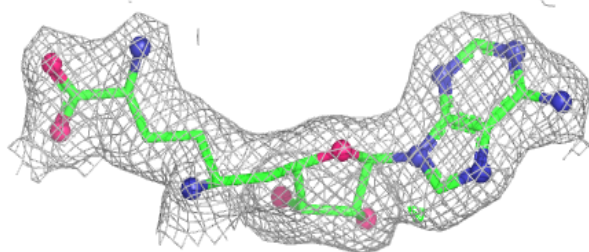
Electron density around SFG B 402:

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 SFG A 401:

$2mF_o-DF_c$ (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.