



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:08 PM UTC

PDB ID : 3TM5 / pdb_00003tm5
Title : Crystal structure of Trm14 from *Pyrococcus furiosus* in complex with sinefungin
Authors : Fislage, M.; Roovers, M.; Tuszynska, I.; Bujnicki, J.M.; Droogmans, L.; Versees, W.
Deposited on : 2011-08-31
Resolution : 2.27 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

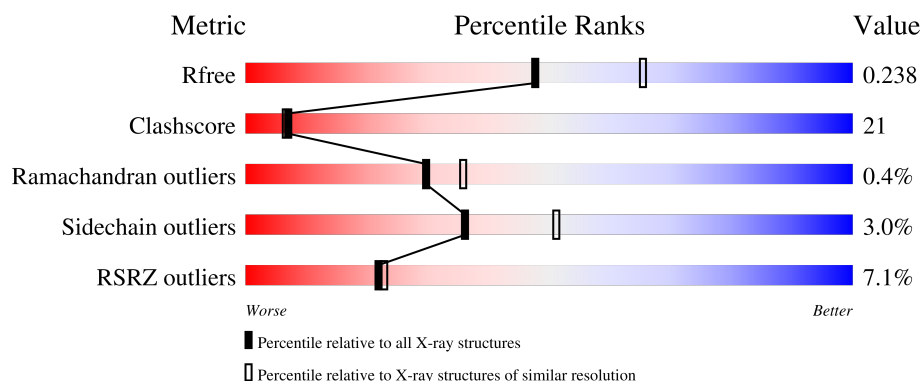
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	373	9% 61% 35% ..
1	B	373	5% 67% 29% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6163 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.

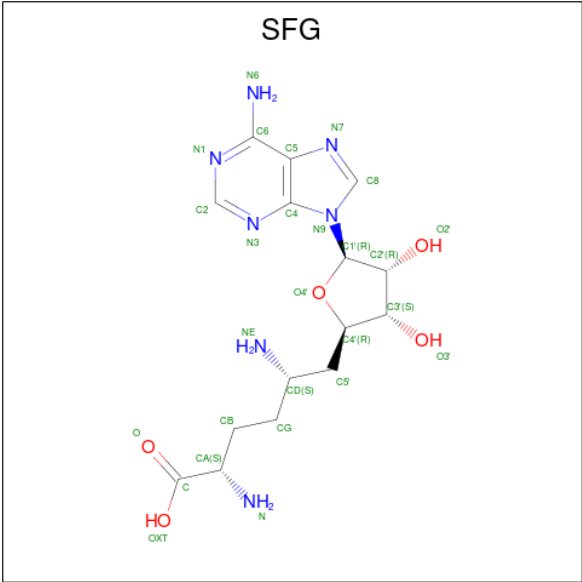
- Molecule 1 is a protein called Crystal structure of Trm14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	2	1	0
			2921	1876	500	537	8			
1	B	368	Total	C	N	O	S	0	3	0
			2935	1888	502	536	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	LEU	-	expression tag	UNP Q8U248
A	367	GLU	-	expression tag	UNP Q8U248
A	368	HIS	-	expression tag	UNP Q8U248
A	369	HIS	-	expression tag	UNP Q8U248
A	370	HIS	-	expression tag	UNP Q8U248
A	371	HIS	-	expression tag	UNP Q8U248
A	372	HIS	-	expression tag	UNP Q8U248
A	373	HIS	-	expression tag	UNP Q8U248
B	366	LEU	-	expression tag	UNP Q8U248
B	367	GLU	-	expression tag	UNP Q8U248
B	368	HIS	-	expression tag	UNP Q8U248
B	369	HIS	-	expression tag	UNP Q8U248
B	370	HIS	-	expression tag	UNP Q8U248
B	371	HIS	-	expression tag	UNP Q8U248
B	372	HIS	-	expression tag	UNP Q8U248
B	373	HIS	-	expression tag	UNP Q8U248

- Molecule 2 is SINEFUNGIN (CCD ID: SFG) (formula: C₁₅H₂₃N₇O₅).



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

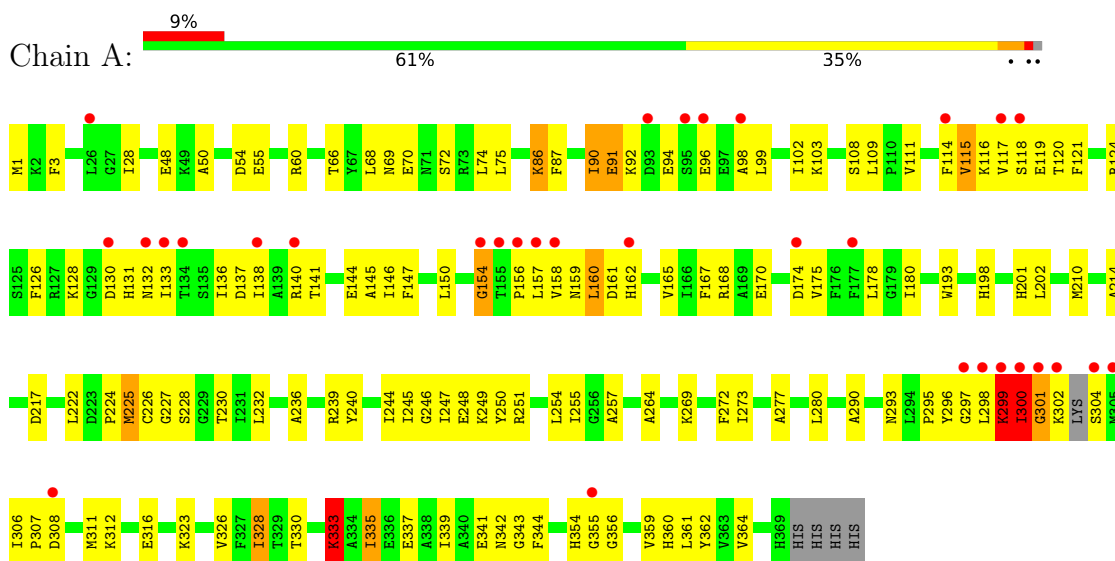
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	122	Total	O	0	0
			122	122		

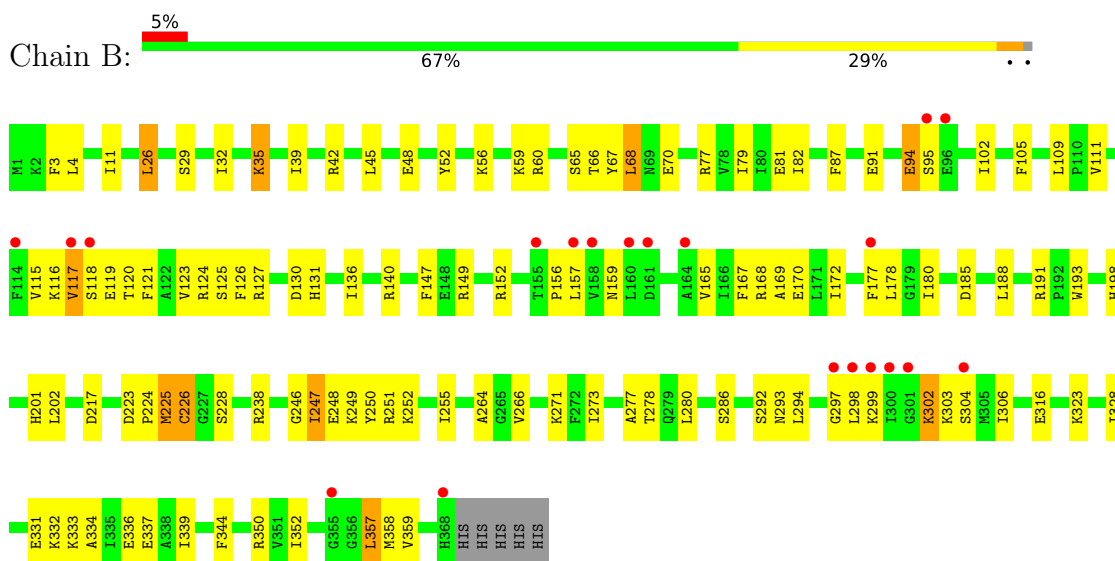
3 Residue-property plots [i](#)

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: Crystal structure of Trm14



• Molecule 1: Crystal structure of Trm14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.25Å 45.06Å 121.08Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	48.02 – 2.27 48.02 – 2.27	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.02-2.27) 99.1 (48.02-2.27)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.219 0.218 , 0.238	Depositor DCC
R_{free} test set	2089 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.086 for h,-k,-l	Xtriage
Reported twinning fraction	0.834 for H, K, L 0.166 for -h,-k,l	Depositor
Outliers	0 of 42271 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6163	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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

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	0.86	3/2974 (0.1%)	1.06	8/3999 (0.2%)
1	B	0.85	1/2994 (0.0%)	1.10	12/4025 (0.3%)
All	All	0.85	4/5968 (0.1%)	1.08	20/8024 (0.2%)

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	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	VAL	N-CA	-5.41	1.40	1.46
1	A	333	LYS	C-O	-5.39	1.17	1.24
1	B	266	VAL	CA-CB	5.19	1.61	1.54
1	A	115	VAL	CA-CB	-5.05	1.47	1.55

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	302	LYS	N-CA-C	-8.22	96.89	109.14
1	B	304	SER	N-CA-C	-7.80	103.73	113.55
1	B	225	MET	CA-C-N	7.32	132.93	120.71
1	B	225	MET	C-N-CA	7.32	132.93	120.71
1	B	226	CYS	N-CA-CB	-6.82	100.04	110.13
1	A	335	ILE	N-CA-C	6.27	116.44	110.42
1	A	180	ILE	CB-CA-C	-5.62	104.12	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	102	ILE	N-CA-C	-5.60	105.27	110.53
1	B	35	LYS	CA-C-N	-5.54	114.06	119.76
1	B	35	LYS	C-N-CA	-5.54	114.06	119.76
1	A	301	GLY	N-CA-C	-5.43	100.30	113.18
1	B	286	SER	CB-CA-C	5.42	119.61	109.86
1	A	158	VAL	CB-CA-C	-5.34	103.45	110.98
1	B	334	ALA	N-CA-C	5.31	117.48	111.11
1	A	91	GLU	N-CA-C	-5.22	106.86	113.18
1	A	90	ILE	N-CA-C	5.14	115.86	110.62
1	A	154	GLY	N-CA-C	5.09	116.81	110.29
1	B	238	ARG	N-CA-C	-5.03	106.98	113.02
1	B	294	LEU	N-CA-C	5.03	116.83	109.84
1	A	158	VAL	N-CA-C	5.01	116.17	108.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	354	HIS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2921	0	3004	141	0
1	B	2935	0	3039	115	0
2	A	27	0	22	2	0
2	B	27	0	22	2	0
3	A	131	0	0	6	0
3	B	122	0	0	14	0
All	All	6163	0	6087	252	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 21.

All (252) 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:225:MET:CE	1:A:295:PRO:HD3	1.52	1.40
1:A:225:MET:HE1	1:A:295:PRO:CD	1.62	1.28
1:A:90:ILE:HG22	1:A:174:ASP:OD1	1.39	1.19
1:B:4:LEU:HD21	1:B:42:ARG:NH2	1.57	1.16
1:B:52:TYR:OH	1:B:60:ARG:HD2	1.46	1.15
1:B:177:PHE:HB3	3:B:605:HOH:O	1.41	1.14
1:A:120:THR:HG21	1:A:159:ASN:HB3	1.35	1.06
1:A:120:THR:HG21	1:A:159:ASN:CB	1.85	1.05
1:B:332:LYS:O	1:B:336:GLU:HG2	1.54	1.05
1:B:247:ILE:HD12	1:B:273:ILE:HB	1.41	1.03
1:A:302:LYS:HD3	3:B:502:HOH:O	1.60	1.02
1:A:120:THR:CG2	1:A:159:ASN:HB3	1.91	1.01
1:B:4:LEU:HD21	1:B:42:ARG:HH21	1.08	1.00
1:A:225:MET:HE1	1:A:295:PRO:HD3	1.00	0.98
1:A:300:ILE:CG1	1:A:301:GLY:H	1.76	0.98
1:B:328:ILE:HG23	1:B:359:VAL:CG1	1.97	0.95
1:B:32:ILE:HD11	1:B:45:LEU:HD13	1.49	0.95
1:B:302:LYS:O	1:B:303:LYS:HB2	1.65	0.94
1:A:91:GLU:HB2	1:A:130:ASP:O	1.67	0.93
1:B:328:ILE:CG2	1:B:359:VAL:HG11	1.98	0.93
1:A:339:ILE:HD11	1:A:364:VAL:HG11	1.47	0.93
1:A:225:MET:HE2	1:A:295:PRO:HD3	1.49	0.90
1:A:339:ILE:CD1	1:A:364:VAL:HG11	2.02	0.90
1:A:228:SER:HB3	2:A:401:SFG:OXT	1.72	0.89
1:B:94:GLU:HG2	1:B:95:SER:N	1.86	0.88
1:B:52:TYR:OH	1:B:60:ARG:CD	2.22	0.86
1:B:306:ILE:HG21	1:B:331:GLU:HG3	1.57	0.86
1:A:133:ILE:HD11	1:A:138:ILE:HD11	1.57	0.85
1:B:298:LEU:HD11	1:B:357:LEU:HD21	1.59	0.85
1:A:311:MET:HE1	1:A:341:GLU:HB2	1.59	0.84
1:B:66:THR:O	1:B:70:GLU:HG2	1.78	0.82
1:A:225:MET:HE1	1:A:295:PRO:CG	2.10	0.81
1:B:246:GLY:C	1:B:247:ILE:HD13	2.06	0.80
1:A:120:THR:CG2	1:A:159:ASN:CB	2.55	0.80
1:B:94:GLU:HG2	1:B:95:SER:H	1.44	0.79
1:A:217:ASP:OD2	1:A:323:LYS:NZ	2.14	0.79
1:A:301:GLY:HA2	1:A:302:LYS:C	2.06	0.79
1:B:109:LEU:CD1	1:B:178:LEU:HD23	2.14	0.78
1:B:127:ARG:HH11	1:B:131:HIS:HD2	1.31	0.77
1:B:332:LYS:O	1:B:336:GLU:CG	2.32	0.77
1:A:298:LEU:O	1:A:299:LYS:HB2	1.83	0.77
1:A:90:ILE:CG2	1:A:174:ASP:OD1	2.27	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:O	1:A:140:ARG:HG3	1.84	0.76
1:A:236:ALA:HB1	1:A:269:LYS:HE3	1.68	0.75
1:A:300:ILE:HG12	1:A:301:GLY:H	1.48	0.75
1:A:333:LYS:NZ	1:A:337:GLU:OE2	2.19	0.75
1:A:300:ILE:CG1	1:A:301:GLY:N	2.49	0.75
1:A:198:HIS:HB2	1:A:228:SER:HB2	1.68	0.75
1:A:308:ASP:O	1:A:312:LYS:HD2	1.87	0.74
1:B:358[A]:MET:HE1	3:B:505:HOH:O	1.89	0.73
1:B:247:ILE:CD1	1:B:273:ILE:HB	2.18	0.73
1:A:120:THR:HG21	1:A:159:ASN:HB2	1.69	0.72
1:A:133:ILE:CD1	1:A:138:ILE:HD11	2.18	0.72
1:B:226:CYS:HB3	1:B:248:GLU:HB2	1.70	0.71
1:B:328:ILE:HG23	1:B:359:VAL:HG12	1.69	0.71
1:B:109:LEU:HD12	1:B:178:LEU:HD23	1.72	0.71
1:A:328:ILE:HG23	1:A:359:VAL:HG11	1.72	0.71
1:A:147:PHE:CE1	1:A:156:PRO:HB2	2.26	0.70
1:A:311:MET:HE1	1:A:341:GLU:CB	2.21	0.70
1:B:226:CYS:HB2	1:B:247:ILE:O	1.91	0.70
1:B:177:PHE:HE1	3:B:511:HOH:O	1.73	0.69
1:B:297:GLY:O	1:B:303:LYS:HG3	1.92	0.69
1:B:32:ILE:CD1	1:B:45:LEU:HD13	2.21	0.69
1:B:4:LEU:CD2	1:B:42:ARG:NH2	2.48	0.69
1:A:280:LEU:HB3	1:A:316:GLU:HB3	1.73	0.68
1:B:328:ILE:HG23	1:B:359:VAL:HG11	1.60	0.68
1:A:300:ILE:HG13	1:A:301:GLY:H	1.57	0.67
1:B:246:GLY:O	1:B:247:ILE:HD13	1.95	0.67
1:B:168:ARG:HD3	3:B:536:HOH:O	1.94	0.67
1:B:328:ILE:CG2	1:B:359:VAL:CG1	2.65	0.67
1:A:210:MET:SD	1:A:328:ILE:HD12	2.35	0.67
1:B:29:SER:HB2	1:B:48:GLU:HG3	1.78	0.66
1:A:54:ASP:OD2	1:A:60:ARG:HD2	1.95	0.66
1:B:136:ILE:O	1:B:140:ARG:HG3	1.96	0.66
1:B:177:PHE:CB	3:B:605:HOH:O	2.17	0.66
1:B:115:VAL:HG23	1:B:165:VAL:HG21	1.78	0.65
1:A:124:ARG:NH2	1:A:160:LEU:O	2.27	0.65
1:B:91:GLU:HG2	1:B:130:ASP:O	1.95	0.65
1:B:4:LEU:HD11	1:B:42:ARG:HD3	1.79	0.65
1:A:302:LYS:HG2	1:B:250:TYR:HD1	1.62	0.65
1:A:116:LYS:O	1:A:117:VAL:C	2.40	0.64
1:A:335:ILE:HG21	1:A:362:TYR:CE2	2.31	0.64
1:A:301:GLY:HA2	1:A:302:LYS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:THR:O	1:B:316:GLU:HG3	1.98	0.63
1:A:193:TRP:CB	1:A:264:ALA:HB2	2.29	0.63
1:B:35:LYS:HB3	1:B:39:ILE:O	1.99	0.62
1:A:198:HIS:HB3	1:A:201:HIS:HB3	1.81	0.62
1:A:254:LEU:HD11	1:A:272:PHE:HB3	1.82	0.62
1:B:52:TYR:CZ	1:B:60:ARG:HD2	2.34	0.62
1:B:125:SER:HA	1:B:169:ALA:O	1.99	0.62
1:B:247:ILE:HD13	1:B:247:ILE:N	2.10	0.61
1:B:188:LEU:O	1:B:191:ARG:NH1	2.34	0.61
1:B:77:ARG:NH2	3:B:573:HOH:O	2.32	0.60
1:A:311:MET:HE3	1:A:342:ASN:HD21	1.66	0.60
1:A:306:ILE:HB	1:A:307:PRO:HD3	1.83	0.60
1:B:280:LEU:HB3	1:B:316:GLU:HB3	1.84	0.59
1:B:302:LYS:O	1:B:303:LYS:CB	2.45	0.59
1:A:300:ILE:CG2	1:B:252:LYS:HE3	2.32	0.59
1:A:361:LEU:C	1:A:361:LEU:HD23	2.29	0.58
1:A:133:ILE:CD1	1:A:138:ILE:CD1	2.81	0.58
1:A:114:PHE:C	1:A:115:VAL:HG13	2.30	0.57
1:A:114:PHE:C	1:A:115:VAL:CG1	2.78	0.57
1:B:147:PHE:CE1	1:B:156:PRO:HG2	2.40	0.57
1:B:249:LYS:HE3	1:B:250:TYR:CZ	2.40	0.56
1:A:299:LYS:HE3	1:B:252:LYS:NZ	2.20	0.56
1:A:301:GLY:CA	1:A:302:LYS:HB3	2.35	0.56
1:A:133:ILE:HD11	1:A:138:ILE:CD1	2.34	0.56
1:A:28:ILE:HD11	1:A:50:ALA:HA	1.89	0.55
1:A:98:ALA:O	1:A:102:ILE:HG12	2.07	0.55
1:A:228:SER:O	1:A:257:ALA:HA	2.07	0.54
1:A:1:MET:HE2	1:A:3:PHE:CZ	2.43	0.54
1:B:126:PHE:O	1:B:170:GLU:HA	2.07	0.54
1:A:225:MET:HE1	1:A:295:PRO:HG3	1.87	0.54
1:A:277:ALA:O	1:A:280:LEU:HB2	2.08	0.54
1:B:177:PHE:CE1	3:B:511:HOH:O	2.53	0.54
1:A:120:THR:HA	1:A:157:LEU:O	2.07	0.53
1:A:160:LEU:HD22	1:A:160:LEU:H	1.73	0.53
1:A:300:ILE:HG13	1:A:301:GLY:N	2.17	0.53
1:A:193:TRP:HB2	1:A:264:ALA:HB2	1.90	0.53
1:B:42:ARG:CZ	1:B:177:PHE:CE1	2.92	0.53
1:A:339:ILE:HD12	1:A:364:VAL:HG11	1.86	0.53
1:B:11[A]:ILE:HD11	1:B:352:ILE:HD13	1.91	0.53
1:B:117:VAL:O	1:B:118:SER:OG	2.23	0.52
1:A:301:GLY:CA	1:A:302:LYS:C	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:HD21	1:A:137:ASP:HB3	1.91	0.52
1:B:109:LEU:HD12	1:B:178:LEU:CD2	2.38	0.52
1:A:120:THR:HG22	1:A:159:ASN:HB3	1.88	0.52
1:A:94:GLU:HA	1:A:132:ASN:HD22	1.75	0.51
1:B:120:THR:HA	1:B:157:LEU:O	2.10	0.51
1:A:115:VAL:HG11	1:A:167:PHE:CZ	2.45	0.51
1:B:42:ARG:NH1	1:B:170:GLU:OE1	2.43	0.51
1:A:99:LEU:HD22	1:A:141:THR:OG1	2.11	0.51
1:A:161:ASP:C	1:A:162:HIS:HD2	2.19	0.51
1:A:343:GLY:HA2	3:A:620:HOH:O	2.11	0.51
1:A:296:TYR:HB3	1:A:330:THR:OG1	2.12	0.50
1:B:4:LEU:CD2	1:B:42:ARG:HH21	2.00	0.50
1:A:54:ASP:HB3	1:A:60:ARG:HD3	1.94	0.50
1:A:293:ASN:HD22	1:A:328:ILE:HG22	1.76	0.50
1:B:198:HIS:HB2	1:B:228:SER:HB3	1.94	0.50
1:A:120:THR:HG22	1:A:121:PHE:N	2.28	0.49
1:B:293:ASN:HB3	2:B:401:SFG:HN2	1.76	0.49
1:B:247:ILE:HD11	1:B:273:ILE:HD12	1.95	0.49
1:A:66:THR:O	1:A:70:GLU:HG2	2.12	0.49
1:B:178:LEU:N	3:B:605:HOH:O	2.45	0.49
1:B:126:PHE:HE2	1:B:172:ILE:HD11	1.76	0.49
2:B:401:SFG:NE	3:B:606:HOH:O	2.35	0.49
1:A:297:GLY:HA3	1:A:306:ILE:HD11	1.95	0.49
1:B:202:LEU:HD22	1:B:293:ASN:HB2	1.95	0.49
1:A:133:ILE:HD12	1:A:138:ILE:CD1	2.43	0.48
1:B:271:LYS:HE2	1:B:273:ILE:HD11	1.96	0.48
1:B:249:LYS:HE3	1:B:250:TYR:OH	2.13	0.48
1:A:116:LYS:C	1:A:118:SER:N	2.71	0.48
1:A:55:GLU:OE1	1:A:55:GLU:N	2.32	0.48
1:A:161:ASP:O	1:A:162:HIS:HD2	1.97	0.48
1:A:224:PRO:O	1:A:247:ILE:O	2.32	0.48
1:B:109:LEU:HD13	1:B:178:LEU:HD23	1.96	0.48
1:A:120:THR:CG2	1:A:159:ASN:HB2	2.36	0.48
1:A:86:LYS:HD2	1:A:175:VAL:HG22	1.95	0.47
1:B:4:LEU:HD21	1:B:42:ARG:HH22	1.65	0.47
1:A:68:LEU:O	1:A:69:ASN:C	2.57	0.47
1:A:226:CYS:SG	1:A:248:GLU:HB2	2.54	0.47
1:A:299:LYS:HE3	1:B:252:LYS:HZ3	1.76	0.47
1:A:255:ILE:CD1	3:A:502:HOH:O	2.62	0.47
1:B:224:PRO:HD2	1:B:292:SER:HB2	1.97	0.47
1:B:226:CYS:CB	1:B:247:ILE:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:HB3	1:A:131:HIS:CD2	2.49	0.47
1:B:121:PHE:CD1	1:B:121:PHE:C	2.92	0.47
1:A:124:ARG:O	1:A:168:ARG:HA	2.14	0.47
1:B:117:VAL:O	1:B:118:SER:CB	2.61	0.47
1:A:116:LYS:O	1:A:118:SER:N	2.48	0.47
1:B:111:VAL:HG22	1:B:167:PHE:CZ	2.49	0.46
1:A:111:VAL:HG12	1:A:150:LEU:HD11	1.98	0.46
1:A:225:MET:HE3	2:A:401:SFG:O4'	2.15	0.46
1:B:65:SER:HB3	3:B:515:HOH:O	2.14	0.46
1:B:225:MET:HE2	1:B:277:ALA:HB3	1.98	0.46
1:A:136:ILE:HG22	1:A:140:ARG:NE	2.31	0.46
1:B:94:GLU:CG	1:B:95:SER:H	2.22	0.46
1:A:87:PHE:N	1:A:87:PHE:CD1	2.84	0.46
1:B:11[A]:ILE:HD11	1:B:352:ILE:CD1	2.46	0.46
1:B:168:ARG:CD	3:B:536:HOH:O	2.60	0.46
1:B:120:THR:HG22	1:B:157:LEU:HB3	1.98	0.45
1:B:193:TRP:CD1	3:B:522:HOH:O	2.69	0.45
1:A:339:ILE:HG23	1:A:344:PHE:HB2	1.99	0.45
1:A:133:ILE:HD12	1:A:138:ILE:HD13	1.97	0.45
1:B:115:VAL:CG2	1:B:165:VAL:HG21	2.43	0.45
1:A:141:THR:HA	1:A:144:GLU:OE1	2.16	0.45
1:B:339:ILE:HG23	1:B:344:PHE:HB2	1.99	0.45
1:A:72:SER:OG	1:A:75:LEU:HG	2.16	0.45
1:A:299:LYS:HD2	1:A:299:LYS:HA	1.51	0.45
1:B:333:LYS:O	1:B:337:GLU:HG3	2.17	0.45
1:A:119:GLU:HB2	3:A:589:HOH:O	2.16	0.45
1:A:128:LYS:O	1:A:131:HIS:HE1	2.00	0.45
1:A:146:ILE:O	1:A:150:LEU:HD13	2.17	0.45
1:A:302:LYS:HE2	1:B:251:ARG:HB2	1.98	0.44
1:A:328:ILE:HG23	1:A:359:VAL:CG1	2.44	0.44
1:B:217:ASP:OD2	1:B:323:LYS:NZ	2.42	0.44
1:B:116:LYS:O	1:B:119:GLU:HB2	2.18	0.44
1:A:87:PHE:N	1:A:87:PHE:HD1	2.15	0.44
1:A:214:ALA:HB2	1:A:326:VAL:HG21	1.99	0.44
1:A:232:LEU:HD11	1:A:246:GLY:CA	2.48	0.44
1:B:111:VAL:CG2	1:B:167:PHE:CE1	3.01	0.44
1:A:161:ASP:C	1:A:162:HIS:CD2	2.96	0.44
1:A:301:GLY:C	1:A:304:SER:HA	2.43	0.44
1:B:120:THR:HB	1:B:159:ASN:HB2	1.99	0.44
1:A:356:GLY:HA2	3:A:621:HOH:O	2.18	0.43
1:B:81:GLU:HG2	1:B:82:ILE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:GLY:HA2	1:A:302:LYS:CB	2.40	0.43
1:A:306:ILE:N	1:A:307:PRO:CD	2.80	0.43
1:B:149:ARG:O	1:B:152[B]:ARG:HG3	2.18	0.43
1:B:198:HIS:HB3	1:B:201:HIS:HB3	2.01	0.43
1:B:124:ARG:NH2	1:B:185:ASP:OD1	2.51	0.43
1:B:193:TRP:CB	1:B:264:ALA:HB2	2.48	0.43
1:A:301:GLY:O	1:A:304:SER:HA	2.18	0.43
1:B:26:LEU:HD13	1:B:67:TYR:CZ	2.54	0.42
1:A:339:ILE:HD12	1:A:364:VAL:CG1	2.48	0.42
1:A:244:ILE:C	1:A:245:ILE:HG13	2.44	0.42
1:A:108[B]:SER:OG	3:A:588:HOH:O	2.21	0.42
1:A:141:THR:HG23	3:A:523:HOH:O	2.19	0.42
1:B:3:PHE:HB2	1:B:45:LEU:HB3	2.00	0.42
1:A:126:PHE:O	1:A:170:GLU:HA	2.20	0.42
1:A:339:ILE:CD1	1:A:364:VAL:CG1	2.88	0.42
1:B:56:LYS:HE3	3:B:571:HOH:O	2.19	0.42
1:B:223:ASP:C	1:B:223:ASP:OD2	2.62	0.42
1:B:299:LYS:HE3	1:B:299:LYS:HB2	1.89	0.42
1:A:109:LEU:CD1	1:A:178:LEU:HD23	2.50	0.42
1:A:222:LEU:O	1:A:290:ALA:HA	2.20	0.41
1:B:123:VAL:HG22	1:B:167:PHE:HB2	2.02	0.41
1:B:251:ARG:HE	1:B:255:ILE:HD11	1.85	0.41
1:A:154:GLY:O	1:A:156:PRO:HD3	2.21	0.41
1:A:239:ARG:O	1:A:240:TYR:C	2.63	0.41
1:A:335:ILE:HD13	1:A:362:TYR:CD2	2.55	0.41
1:A:251:ARG:O	1:A:255:ILE:HG12	2.19	0.41
1:A:147:PHE:CD1	1:A:156:PRO:HB2	2.56	0.41
1:A:202:LEU:O	1:A:230:THR:HG21	2.20	0.41
1:A:86:LYS:HB3	1:A:86:LYS:HE3	1.88	0.41
1:A:249:LYS:HD3	1:A:250:TYR:CZ	2.56	0.41
1:A:293:ASN:HD22	1:A:328:ILE:CG2	2.34	0.41
1:A:328:ILE:HA	1:A:360:HIS:O	2.21	0.41
1:B:68:LEU:HA	1:B:68:LEU:HD12	1.86	0.41
1:B:127:ARG:HH11	1:B:131:HIS:CD2	2.23	0.41
1:B:87:PHE:HZ	1:B:105:PHE:CG	2.39	0.41
1:B:350:ARG:HD2	1:B:352:ILE:HD11	2.02	0.41
1:A:54:ASP:HB3	1:A:60:ARG:CD	2.51	0.40
1:B:32:ILE:CD1	1:B:45:LEU:CD1	2.96	0.40
1:A:103:LYS:HG3	1:A:145:ALA:HB2	2.03	0.40
1:A:109:LEU:HD12	1:A:178:LEU:HD23	2.03	0.40
1:A:247:ILE:HG12	1:A:273:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLY:O	1:A:257:ALA:HB2	2.21	0.40
1:B:4:LEU:HD23	1:B:79:ILE:HD12	2.02	0.40
1:B:167:PHE:CE1	1:B:180:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	365/373 (98%)	352 (96%)	10 (3%)	3 (1%)	16	18
1	B	369/373 (99%)	358 (97%)	11 (3%)	0	100	100
All	All	734/746 (98%)	710 (97%)	21 (3%)	3 (0%)	30	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	LYS
1	A	300	ILE
1	A	355	GLY

5.3.2 Protein sidechains [i](#)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	315/319 (99%)	303 (96%)	12 (4%)	29	42
1	B	317/319 (99%)	310 (98%)	7 (2%)	45	62
All	All	632/638 (99%)	613 (97%)	19 (3%)	36	51

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	74	LEU
1	A	86	LYS
1	A	92	LYS
1	A	96	GLU
1	A	160	LEU
1	A	165	VAL
1	A	225	MET
1	A	299	LYS
1	A	300	ILE
1	A	328	ILE
1	A	333	LYS
1	B	26	LEU
1	B	59	LYS
1	B	68	LEU
1	B	94	GLU
1	B	117	VAL
1	B	247	ILE
1	B	357	LEU

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	9	GLN
1	A	131	HIS
1	A	132	ASN
1	A	162	HIS
1	A	253	HIS
1	A	293	ASN
1	A	342	ASN
1	B	69	ASN

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Mol	Chain	Res	Type
1	B	131	HIS
1	B	293	ASN
1	B	315	ASN
1	B	354	HIS
1	B	368	HIS

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SFG	B	401	-	28,29,29	1.51	6 (21%)	34,42,42	2.33	13 (38%)
2	SFG	A	401	-	28,29,29	1.51	5 (17%)	34,42,42	2.03	9 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SFG	B	401	-	-	9/17/33/33	0/3/3/3
2	SFG	A	401	-	-	2/17/33/33	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SFG	C5-C4	4.79	1.47	1.39
2	B	401	SFG	C5-C4	4.67	1.47	1.39
2	A	401	SFG	C5-N7	-3.39	1.32	1.39
2	B	401	SFG	C5-N7	-2.98	1.33	1.39
2	B	401	SFG	C5-C6	2.74	1.48	1.41
2	A	401	SFG	C4-N9	-2.65	1.32	1.37
2	B	401	SFG	C4-N9	-2.35	1.32	1.37
2	A	401	SFG	C5-C6	2.34	1.47	1.41
2	B	401	SFG	OXT-C	-2.25	1.23	1.30
2	B	401	SFG	C8-N7	2.15	1.35	1.31
2	A	401	SFG	C8-N7	2.05	1.35	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SFG	C5-C4-N3	-6.42	117.88	126.72
2	B	401	SFG	C5-C4-N3	-6.05	118.39	126.72
2	A	401	SFG	N3-C4-N9	4.82	135.36	127.17
2	B	401	SFG	N3-C4-N9	4.55	134.91	127.17
2	B	401	SFG	OXT-C-O	-4.39	114.12	124.08
2	B	401	SFG	O4'-C1'-N9	3.98	115.73	108.09
2	B	401	SFG	C2-N3-C4	3.81	121.13	111.83
2	B	401	SFG	C4-C5-N7	-3.70	106.35	110.58
2	A	401	SFG	C2-N3-C4	3.62	120.67	111.83
2	A	401	SFG	C4-C5-N7	-3.34	106.76	110.58
2	B	401	SFG	N3-C2-N1	-3.18	123.76	128.58
2	B	401	SFG	C5-N7-C8	2.82	107.88	103.45
2	A	401	SFG	N3-C2-N1	-2.69	124.51	128.58
2	A	401	SFG	O4'-C1'-N9	2.39	112.69	108.09
2	B	401	SFG	CG-CD-C5'	2.39	117.77	111.08
2	B	401	SFG	C4-N9-C8	2.34	108.19	105.74
2	A	401	SFG	OXT-C-O	-2.33	118.79	124.08
2	B	401	SFG	C6-C5-N7	2.23	136.38	132.09
2	A	401	SFG	C5-N7-C8	2.22	106.94	103.45
2	B	401	SFG	N9-C8-N7	-2.19	110.83	113.94
2	B	401	SFG	O4'-C4'-C5'	2.17	113.17	109.41
2	A	401	SFG	O4'-C1'-C2'	-2.01	102.32	106.62

There are no chirality outliers.

All (11) torsion outliers are listed below:

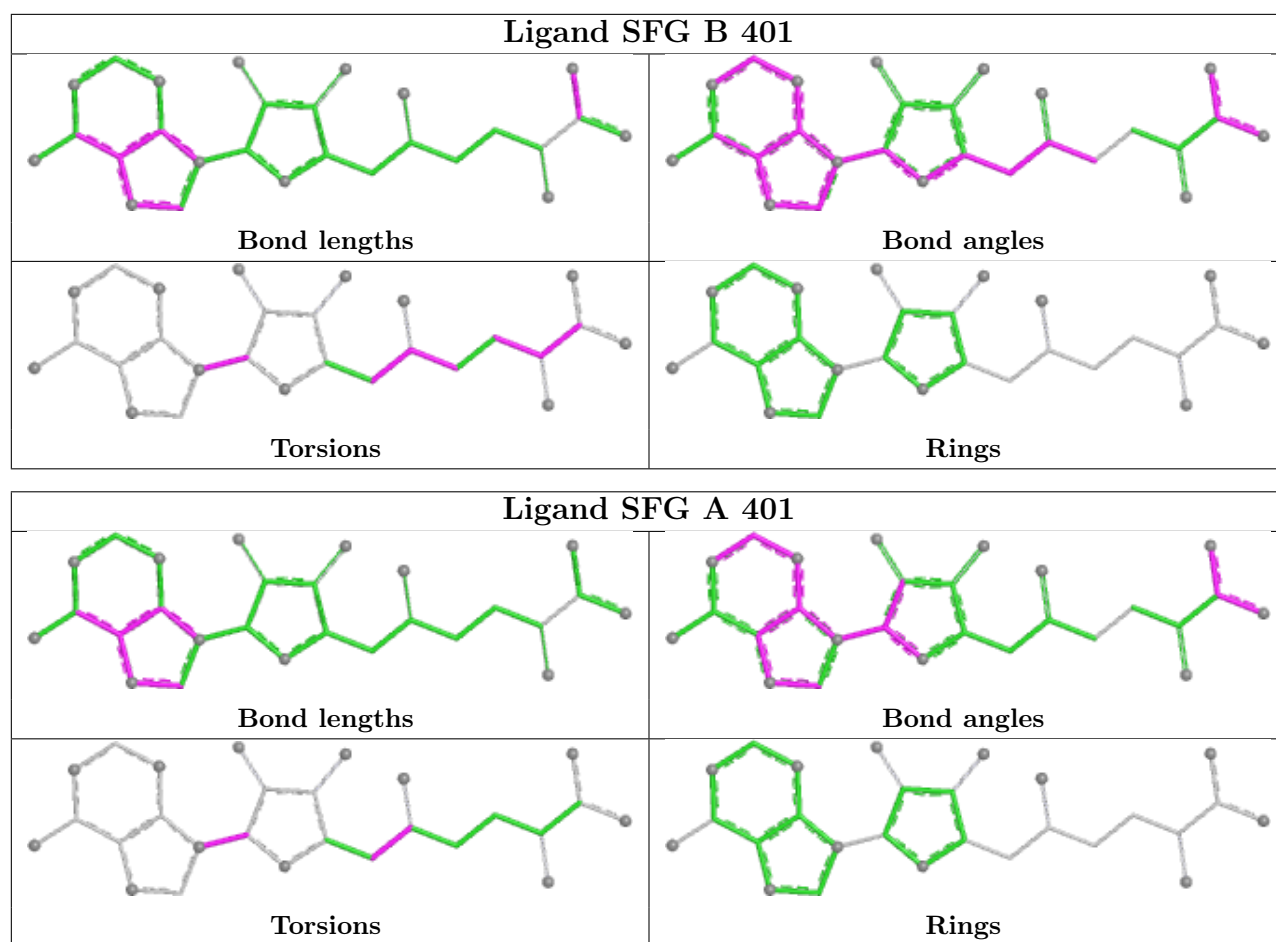
Mol	Chain	Res	Type	Atoms
2	B	401	SFG	N-CA-CB-CG
2	B	401	SFG	C-CA-CB-CG
2	B	401	SFG	C5'-CD-CG-CB
2	B	401	SFG	C2'-C1'-N9-C8
2	B	401	SFG	OXT-C-CA-CB
2	B	401	SFG	NE-CD-CG-CB
2	B	401	SFG	O-C-CA-CB
2	B	401	SFG	O-C-CA-N
2	A	401	SFG	C2'-C1'-N9-C8
2	A	401	SFG	C4'-C5'-CD-NE
2	B	401	SFG	C4'-C5'-CD-NE

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SFG	2	0
2	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	368/373 (98%)	0.57	32 (8%) 16 16	7, 23, 46, 58	2 (0%)
1	B	368/373 (98%)	0.39	20 (5%) 31 32	6, 21, 45, 55	3 (0%)
All	All	736/746 (98%)	0.48	52 (7%) 22 23	6, 22, 46, 58	5 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	ILE	7.2
1	B	300	ILE	5.2
1	B	157	LEU	4.6
1	A	301	GLY	4.1
1	B	301	GLY	3.7
1	A	298	LEU	3.7
1	A	140	ARG	3.7
1	A	117	VAL	3.5
1	B	160	LEU	3.5
1	A	158	VAL	3.4
1	A	157	LEU	3.4
1	A	133	ILE	3.3
1	A	130	ASP	3.3
1	B	299	LYS	3.3
1	A	93	ASP	3.3
1	B	117	VAL	3.3
1	B	298	LEU	3.2
1	A	302	LYS	3.1
1	A	299	LYS	3.1
1	B	155	THR	3.1
1	A	174	ASP	3.0
1	A	355	GLY	3.0
1	B	118	SER	2.8
1	A	96	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	95	SER	2.7
1	B	297	GLY	2.6
1	A	26	LEU	2.6
1	A	297	GLY	2.6
1	B	158	VAL	2.6
1	A	114	PHE	2.5
1	B	95	SER	2.5
1	A	98	ALA	2.5
1	B	164	ALA	2.5
1	A	155	THR	2.4
1	B	177	PHE	2.4
1	B	96	GLU	2.4
1	A	138	ILE	2.3
1	B	368	HIS	2.3
1	B	355	GLY	2.3
1	B	161	ASP	2.3
1	A	162	HIS	2.2
1	A	305	MET	2.2
1	A	118	SER	2.2
1	A	304	SER	2.2
1	A	308	ASP	2.2
1	A	177	PHE	2.1
1	B	114	PHE	2.1
1	A	154	GLY	2.1
1	A	134	THR	2.1
1	A	132	ASN	2.0
1	A	156	PRO	2.0
1	B	304	SER	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,

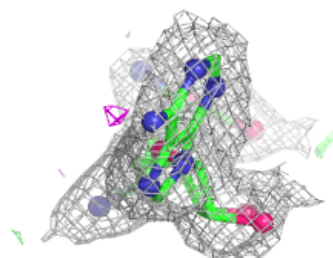
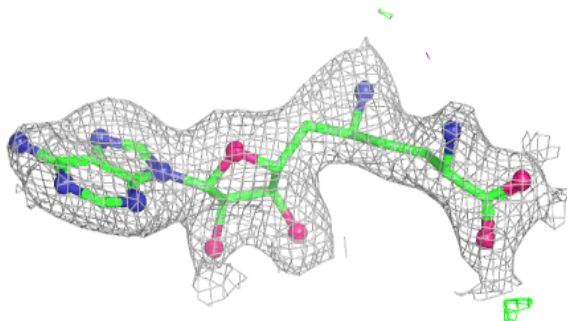
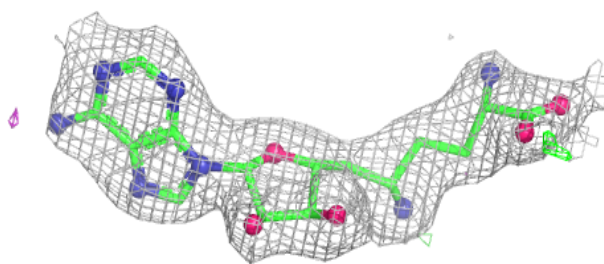
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SFG	A	401	27/27	0.91	0.10	14,18,23,24	0
2	SFG	B	401	27/27	0.92	0.08	11,16,18,21	0

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

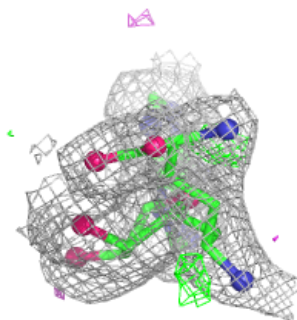
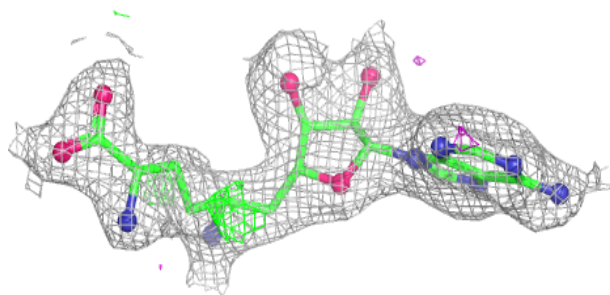
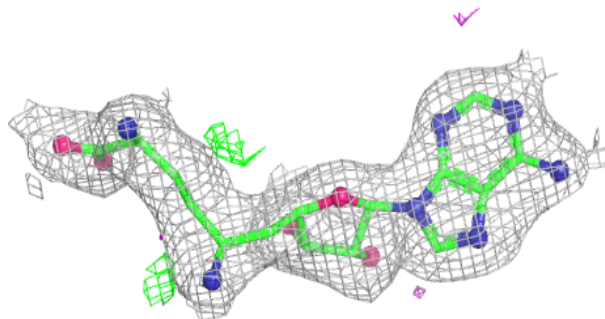
Electron density around SFG A 401:

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



Electron density around SFG B 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.