



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:31 PM UTC

PDB ID : 7Q34 / pdb_00007q34
Title : Crystal structure of the multidrug binding transcriptional regulator LmrR in complex squaraine dye
Authors : Liutkus, M.; Mejias, S.H.; Barolo, C.; Cortajarena, A.L.
Deposited on : 2021-10-26
Resolution : 2.60 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

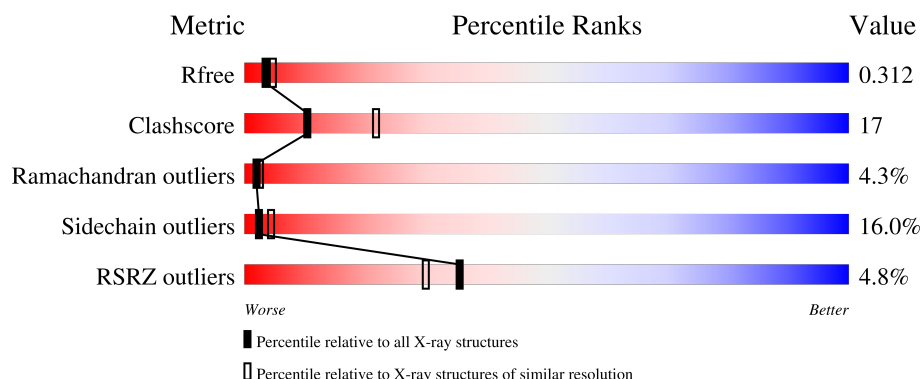
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	132	2% 52%19%5%23%
1	B	132	5% 37%29%8%26%
1	C	132	2% 45%27%7%20%
1	D	132	5% 35%23%9%33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3252 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 Helix-turn-helix transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	101	Total	C	N	O	S	0	0	0
			822	516	142	161	3			
1	B	98	Total	C	N	O	S	0	0	0
			797	504	135	155	3			
1	C	105	Total	C	N	O	S	0	1	0
			856	535	148	170	3			
1	D	88	Total	C	N	O	S	0	0	0
			705	440	123	139	3			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A0A7SZD7
A	1	GLY	-	expression tag	UNP A0A0A7SZD7
A	55	ASP	LYS	conflict	UNP A0A0A7SZD7
A	59	GLN	LYS	conflict	UNP A0A0A7SZD7
A	67	ALA	TRP	conflict	UNP A0A0A7SZD7
A	101	LYS	GLU	conflict	UNP A0A0A7SZD7
A	112	SER	-	expression tag	UNP A0A0A7SZD7
A	113	GLU	-	expression tag	UNP A0A0A7SZD7
A	114	ALA	-	expression tag	UNP A0A0A7SZD7
A	115	ILE	-	expression tag	UNP A0A0A7SZD7
A	116	LYS	-	expression tag	UNP A0A0A7SZD7
A	117	SER	-	expression tag	UNP A0A0A7SZD7
A	118	ARG	-	expression tag	UNP A0A0A7SZD7
A	119	GLY	-	expression tag	UNP A0A0A7SZD7
A	120	GLY	-	expression tag	UNP A0A0A7SZD7
A	121	SER	-	expression tag	UNP A0A0A7SZD7
A	122	GLY	-	expression tag	UNP A0A0A7SZD7
A	123	GLY	-	expression tag	UNP A0A0A7SZD7
A	124	ALA	-	expression tag	UNP A0A0A7SZD7
A	125	SER	-	expression tag	UNP A0A0A7SZD7
A	126	HIS	-	expression tag	UNP A0A0A7SZD7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	127	PRO	-	expression tag	UNP A0A0A7SZD7
A	128	GLN	-	expression tag	UNP A0A0A7SZD7
A	129	PHE	-	expression tag	UNP A0A0A7SZD7
A	130	GLU	-	expression tag	UNP A0A0A7SZD7
A	131	LYS	-	expression tag	UNP A0A0A7SZD7
B	0	MET	-	initiating methionine	UNP A0A0A7SZD7
B	1	GLY	-	expression tag	UNP A0A0A7SZD7
B	55	ASP	LYS	conflict	UNP A0A0A7SZD7
B	59	GLN	LYS	conflict	UNP A0A0A7SZD7
B	67	ALA	TRP	conflict	UNP A0A0A7SZD7
B	101	LYS	GLU	conflict	UNP A0A0A7SZD7
B	112	SER	-	expression tag	UNP A0A0A7SZD7
B	113	GLU	-	expression tag	UNP A0A0A7SZD7
B	114	ALA	-	expression tag	UNP A0A0A7SZD7
B	115	ILE	-	expression tag	UNP A0A0A7SZD7
B	116	LYS	-	expression tag	UNP A0A0A7SZD7
B	117	SER	-	expression tag	UNP A0A0A7SZD7
B	118	ARG	-	expression tag	UNP A0A0A7SZD7
B	119	GLY	-	expression tag	UNP A0A0A7SZD7
B	120	GLY	-	expression tag	UNP A0A0A7SZD7
B	121	SER	-	expression tag	UNP A0A0A7SZD7
B	122	GLY	-	expression tag	UNP A0A0A7SZD7
B	123	GLY	-	expression tag	UNP A0A0A7SZD7
B	124	ALA	-	expression tag	UNP A0A0A7SZD7
B	125	SER	-	expression tag	UNP A0A0A7SZD7
B	126	HIS	-	expression tag	UNP A0A0A7SZD7
B	127	PRO	-	expression tag	UNP A0A0A7SZD7
B	128	GLN	-	expression tag	UNP A0A0A7SZD7
B	129	PHE	-	expression tag	UNP A0A0A7SZD7
B	130	GLU	-	expression tag	UNP A0A0A7SZD7
B	131	LYS	-	expression tag	UNP A0A0A7SZD7
C	0	MET	-	initiating methionine	UNP A0A0A7SZD7
C	1	GLY	-	expression tag	UNP A0A0A7SZD7
C	55	ASP	LYS	conflict	UNP A0A0A7SZD7
C	59	GLN	LYS	conflict	UNP A0A0A7SZD7
C	67	ALA	TRP	conflict	UNP A0A0A7SZD7
C	101	LYS	GLU	conflict	UNP A0A0A7SZD7
C	112	SER	-	expression tag	UNP A0A0A7SZD7
C	113	GLU	-	expression tag	UNP A0A0A7SZD7
C	114	ALA	-	expression tag	UNP A0A0A7SZD7
C	115	ILE	-	expression tag	UNP A0A0A7SZD7
C	116	LYS	-	expression tag	UNP A0A0A7SZD7

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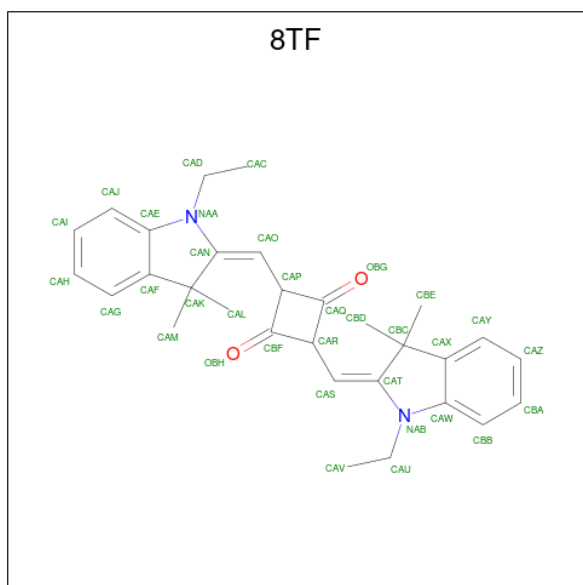
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Chain	Residue	Modelled	Actual	Comment	Reference
C	117	SER	-	expression tag	UNP A0A0A7SZD7
C	118	ARG	-	expression tag	UNP A0A0A7SZD7
C	119	GLY	-	expression tag	UNP A0A0A7SZD7
C	120	GLY	-	expression tag	UNP A0A0A7SZD7
C	121	SER	-	expression tag	UNP A0A0A7SZD7
C	122	GLY	-	expression tag	UNP A0A0A7SZD7
C	123	GLY	-	expression tag	UNP A0A0A7SZD7
C	124	ALA	-	expression tag	UNP A0A0A7SZD7
C	125	SER	-	expression tag	UNP A0A0A7SZD7
C	126	HIS	-	expression tag	UNP A0A0A7SZD7
C	127	PRO	-	expression tag	UNP A0A0A7SZD7
C	128	GLN	-	expression tag	UNP A0A0A7SZD7
C	129	PHE	-	expression tag	UNP A0A0A7SZD7
C	130	GLU	-	expression tag	UNP A0A0A7SZD7
C	131	LYS	-	expression tag	UNP A0A0A7SZD7
D	0	MET	-	initiating methionine	UNP A0A0A7SZD7
D	1	GLY	-	expression tag	UNP A0A0A7SZD7
D	55	ASP	LYS	conflict	UNP A0A0A7SZD7
D	59	GLN	LYS	conflict	UNP A0A0A7SZD7
D	67	ALA	TRP	conflict	UNP A0A0A7SZD7
D	101	LYS	GLU	conflict	UNP A0A0A7SZD7
D	112	SER	-	expression tag	UNP A0A0A7SZD7
D	113	GLU	-	expression tag	UNP A0A0A7SZD7
D	114	ALA	-	expression tag	UNP A0A0A7SZD7
D	115	ILE	-	expression tag	UNP A0A0A7SZD7
D	116	LYS	-	expression tag	UNP A0A0A7SZD7
D	117	SER	-	expression tag	UNP A0A0A7SZD7
D	118	ARG	-	expression tag	UNP A0A0A7SZD7
D	119	GLY	-	expression tag	UNP A0A0A7SZD7
D	120	GLY	-	expression tag	UNP A0A0A7SZD7
D	121	SER	-	expression tag	UNP A0A0A7SZD7
D	122	GLY	-	expression tag	UNP A0A0A7SZD7
D	123	GLY	-	expression tag	UNP A0A0A7SZD7
D	124	ALA	-	expression tag	UNP A0A0A7SZD7
D	125	SER	-	expression tag	UNP A0A0A7SZD7
D	126	HIS	-	expression tag	UNP A0A0A7SZD7
D	127	PRO	-	expression tag	UNP A0A0A7SZD7
D	128	GLN	-	expression tag	UNP A0A0A7SZD7
D	129	PHE	-	expression tag	UNP A0A0A7SZD7
D	130	GLU	-	expression tag	UNP A0A0A7SZD7
D	131	LYS	-	expression tag	UNP A0A0A7SZD7

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ni 2 2	0	0
2	B	2	Total Ni 2 2	0	0

- Molecule 3 is 2,4-bis[(E)-(1-ethyl-3,3-dimethyl-indol-2-ylidene)methyl]cyclobutane-1,3-dione (CCD ID: 8TF) (formula: C₃₀H₃₄N₂O₂) (labeled as "Ligand of Interest" by depositor).

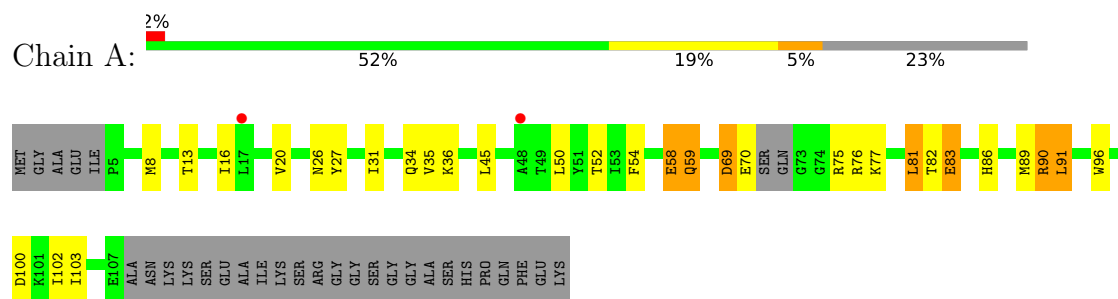


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 34 30 2 2	0	0
3	C	1	Total C N O 34 30 2 2	0	0

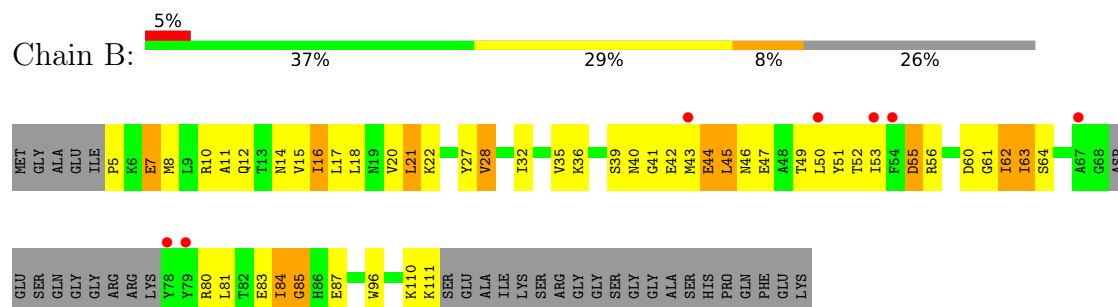
3 Residue-property plots [i](#)

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.

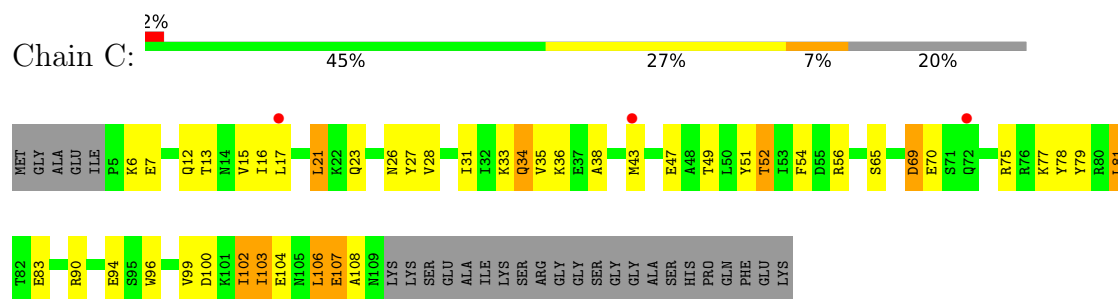
- Molecule 1: Helix-turn-helix transcriptional regulator



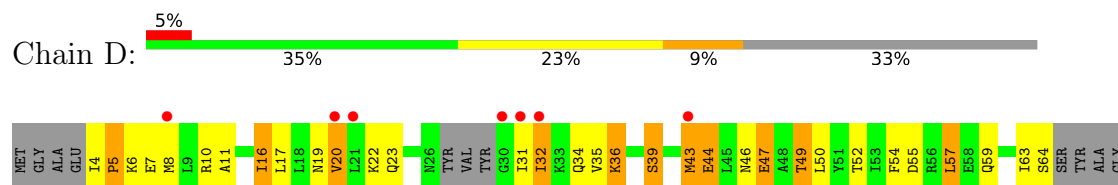
- Molecule 1: Helix-turn-helix transcriptional regulator



- Molecule 1: Helix-turn-helix transcriptional regulator



- Molecule 1: Helix-turn-helix transcriptional regulator



ASP	GLU	SER	GLN	GLY	GLY	ARG	ARG	ARG	LYS	TYR	TYR	R80	I81	T82	E83	E87	N88	M89	W96	K101	I102	N105	N109	LYS	LYS	SER	GLU	ALA	ILE	LYS	SER	SER	ARG	GLY	GLY	SER	GLY	GLY	ALA	SER	HIS	PRO	GLN	PHE	GLU	LYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.66Å 68.02Å 200.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.51 – 2.60 64.51 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.51-2.60) 100.0 (64.51-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.241 , 0.317 0.245 , 0.312	Depositor DCC
R_{free} test set	990 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	74.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3252	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.54% 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: 8TF, NI

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	1.04	1/832 (0.1%)	1.60	6/1115 (0.5%)
1	B	1.06	0/807	1.59	2/1083 (0.2%)
1	C	1.04	0/870	1.58	7/1168 (0.6%)
1	D	1.06	0/709	1.61	1/950 (0.1%)
All	All	1.05	1/3218 (0.0%)	1.59	16/4316 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	HIS	CE1-NE2	5.62	1.38	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	52	THR	CB-CA-C	7.18	122.71	110.86
1	A	83	GLU	CB-CA-C	6.91	121.87	110.81
1	A	83	GLU	CB-CG-CD	6.03	122.84	112.60
1	D	83	GLU	CB-CG-CD	5.74	122.36	112.60
1	A	13	THR	CA-CB-OG1	-5.73	101.00	109.60
1	C	23	GLN	N-CA-C	-5.71	105.20	111.82
1	C	52	THR	N-CA-C	-5.60	104.02	111.24
1	C	49	THR	CA-C-N	5.59	128.09	120.54
1	C	49	THR	C-N-CA	5.59	128.09	120.54
1	C	21	LEU	CA-C-N	5.39	127.50	120.28
1	C	21	LEU	C-N-CA	5.39	127.50	120.28
1	A	82	THR	CA-C-N	5.30	127.70	120.54
1	A	82	THR	C-N-CA	5.30	127.70	120.54
1	B	41	GLY	CA-C-N	5.28	127.61	120.38
1	B	41	GLY	C-N-CA	5.28	127.61	120.38
1	A	83	GLU	N-CA-C	-5.09	105.00	111.11

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	822	0	813	22	0
1	B	797	0	795	43	0
1	C	856	0	844	30	0
1	D	705	0	711	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	34	0	0	5	0
3	C	34	0	0	3	0
All	All	3252	0	3163	109	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 17.

All (109) 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:B:62:ILE:HG22	1:B:85:GLY:HA2	1.30	1.07
1:B:21:LEU:HD12	1:B:63:ILE:HD11	1.47	0.96
1:B:35:VAL:HG11	1:B:45:LEU:HD11	1.52	0.90
1:B:62:ILE:HG22	1:B:85:GLY:CA	2.05	0.85
1:A:96:TRP:CZ2	3:A:203:8TF:CAM	2.64	0.81
1:C:106:LEU:HD21	1:D:20:VAL:HG23	1.65	0.78
1:B:46:ASN:ND2	1:B:49:THR:OG1	2.19	0.76
1:A:35:VAL:HG11	1:A:45:LEU:HD11	1.68	0.75
1:D:57:LEU:O	1:D:59:GLN:O	2.04	0.75
1:B:35:VAL:CG1	1:B:45:LEU:HD11	2.17	0.73
1:C:43:MET:HE2	1:D:102:ILE:HD13	1.76	0.67
1:A:26:ASN:ND2	1:A:34:GLN:OE1	2.30	0.64
1:D:7:GLU:O	1:D:10:ARG:HB3	1.99	0.62
1:C:12:GLN:O	1:C:16:ILE:HG12	1.99	0.62
1:C:26:ASN:HD21	1:C:34:GLN:HE22	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ASN:HB3	1:D:49:THR:OG1	2.00	0.62
1:B:62:ILE:CG2	1:B:85:GLY:HA2	2.18	0.62
1:A:102:ILE:HD13	1:B:43:MET:HG3	1.82	0.61
1:A:69:ASP:OD1	1:A:75:ARG:HG2	2.01	0.61
3:A:203:8TF:CAL	1:B:96:TRP:CZ2	2.84	0.61
1:B:51:TYR:O	1:B:52:THR:OG1	2.15	0.61
1:B:5:PRO:HG2	1:B:8:MET:HE3	1.83	0.60
1:A:102:ILE:CD1	1:B:43:MET:HG3	2.32	0.60
1:B:62:ILE:N	1:B:62:ILE:HD13	2.17	0.60
1:B:21:LEU:HD23	1:B:21:LEU:N	2.16	0.59
1:A:35:VAL:HG11	1:A:45:LEU:CD1	2.31	0.59
1:B:8:MET:O	1:B:12:GLN:HG3	2.02	0.59
1:D:32:ILE:CD1	1:D:50:LEU:HD11	2.32	0.59
1:D:44:GLU:N	1:D:44:GLU:OE1	2.37	0.58
1:B:64:SER:HB2	1:B:80:ARG:HG3	1.86	0.57
1:B:64:SER:HB2	1:B:80:ARG:CG	2.34	0.57
1:C:47:GLU:HG2	1:C:51:TYR:CE2	2.40	0.57
1:C:13:THR:O	1:C:17:LEU:HG	2.04	0.57
1:B:36:LYS:HG3	1:B:45:LEU:CD2	2.37	0.55
3:A:203:8TF:CAL	1:B:96:TRP:CH2	2.89	0.55
1:B:7:GLU:H	1:B:7:GLU:CD	2.13	0.55
1:B:39:SER:O	1:B:42:GLU:HB2	2.06	0.54
1:A:16:ILE:O	1:A:20:VAL:HG23	2.07	0.54
1:D:35:VAL:O	1:D:39:SER:N	2.41	0.54
1:B:51:TYR:C	1:B:52:THR:HG1	2.13	0.54
1:C:28:VAL:HG22	1:C:54:PHE:HE2	1.71	0.54
1:A:81:LEU:HD21	1:A:89:MET:SD	2.49	0.53
1:B:44:GLU:CD	1:B:44:GLU:H	2.16	0.53
1:A:27:TYR:CZ	1:A:76:ARG:NH1	2.77	0.53
1:C:102:ILE:HG22	1:C:103:ILE:N	2.24	0.52
1:C:83[A]:GLU:H	1:C:83[A]:GLU:CD	2.14	0.52
1:A:96:TRP:HZ2	3:A:203:8TF:CAM	2.20	0.52
1:C:38:ALA:O	1:D:105:ASN:ND2	2.43	0.52
1:C:96:TRP:NE1	3:C:201:8TF:CAM	2.73	0.51
1:A:96:TRP:CZ2	1:B:12:GLN:HG2	2.46	0.51
1:B:84:ILE:O	1:B:87:GLU:HB3	2.10	0.51
1:B:16:ILE:O	1:B:20:VAL:HG23	2.11	0.50
1:A:70:GLU:OE2	1:A:70:GLU:N	2.45	0.50
1:C:107:GLU:HA	1:D:23:GLN:NE2	2.26	0.50
1:B:40:ASN:C	1:B:42:GLU:H	2.19	0.50
1:C:99:VAL:HG13	1:D:16:ILE:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:TYR:C	1:A:31:ILE:HD12	2.38	0.49
1:A:100:ASP:OD2	3:A:203:8TF:CAY	2.60	0.49
1:A:90:ARG:NH1	1:A:90:ARG:HB3	2.28	0.49
1:A:54:PHE:O	1:A:58:GLU:HG3	2.13	0.48
1:B:83:GLU:CD	1:B:83:GLU:H	2.21	0.48
1:D:39:SER:HB2	1:D:43:MET:HB2	1.96	0.48
1:D:5:PRO:HD2	1:D:8:MET:HE2	1.96	0.47
1:C:65:SER:HA	1:C:78:TYR:O	2.14	0.47
1:D:35:VAL:CG1	1:D:43:MET:HB3	2.44	0.47
1:C:69:ASP:OD1	1:C:69:ASP:N	2.47	0.47
1:C:43:MET:HE2	1:D:102:ILE:CD1	2.44	0.47
1:C:28:VAL:HG21	1:C:51:TYR:CE1	2.50	0.47
1:D:63:ILE:HA	1:D:82:THR:HG23	1.98	0.45
1:B:14:ASN:O	1:B:18:LEU:HG	2.17	0.45
1:C:38:ALA:HB1	1:D:105:ASN:HB2	1.98	0.45
3:C:201:8TF:CAL	1:D:96:TRP:CH2	2.99	0.45
1:A:27:TYR:O	1:A:31:ILE:HD12	2.16	0.45
1:B:11:ALA:O	1:B:15:VAL:HG23	2.17	0.45
1:C:27:TYR:O	1:C:28:VAL:C	2.60	0.45
1:C:47:GLU:HG2	1:C:51:TYR:HE2	1.82	0.45
1:B:55:ASP:OD2	1:B:55:ASP:N	2.50	0.45
1:C:15:VAL:HG21	3:C:201:8TF:CAL	2.47	0.44
1:C:77:LYS:HE3	1:C:79:TYR:OH	2.18	0.44
1:D:10:ARG:O	1:D:11:ALA:C	2.60	0.44
1:D:32:ILE:O	1:D:35:VAL:HB	2.17	0.44
1:A:96:TRP:CH2	1:B:12:GLN:HG2	2.53	0.44
1:D:50:LEU:HB3	1:D:54:PHE:CE1	2.53	0.43
1:C:21:LEU:HD21	1:C:31:ILE:HD11	2.01	0.43
1:C:90:ARG:NH1	1:C:94:GLU:OE2	2.52	0.43
1:C:35:VAL:CG1	1:C:43:MET:HE3	2.49	0.43
1:D:22:LYS:HD2	1:D:89:MET:HE1	2.00	0.43
1:B:61:GLY:N	1:B:62:ILE:HD13	2.34	0.43
1:D:17:LEU:HD23	1:D:17:LEU:HA	1.89	0.43
1:D:49:THR:O	1:D:52:THR:OG1	2.31	0.43
1:D:64:SER:C	1:D:80:ARG:HB3	2.44	0.42
1:B:27:TYR:O	1:B:28:VAL:C	2.62	0.42
1:B:36:LYS:HG3	1:B:45:LEU:HD22	2.01	0.41
1:B:45:LEU:N	1:B:45:LEU:HD13	2.35	0.41
1:A:59:GLN:NE2	1:C:7:GLU:OE1	2.54	0.41
1:B:43:MET:O	1:B:45:LEU:HD22	2.21	0.41
1:C:81:LEU:HD13	1:C:81:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:ILE:O	1:C:104:GLU:C	2.64	0.41
1:D:32:ILE:O	1:D:36:LYS:NZ	2.49	0.41
1:C:26:ASN:HD21	1:C:34:GLN:NE2	2.13	0.41
1:B:14:ASN:O	1:B:17:LEU:HB2	2.21	0.41
1:B:60:ASP:HB2	1:B:62:ILE:HD11	2.02	0.41
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.88	0.40
1:B:43:MET:O	1:B:45:LEU:HD13	2.21	0.40
1:B:49:THR:O	1:B:53:ILE:HD13	2.21	0.40
1:C:35:VAL:HG11	1:C:43:MET:HE3	2.03	0.40
1:B:84:ILE:O	1:B:87:GLU:N	2.55	0.40
1:B:5:PRO:CG	1:B:8:MET:HE3	2.50	0.40
1:A:91:LEU:HD22	1:A:91:LEU:HA	1.95	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	97/132 (74%)	85 (88%)	12 (12%)	0	100	100
1	B	94/132 (71%)	75 (80%)	13 (14%)	6 (6%)	1	1
1	C	104/132 (79%)	84 (81%)	13 (12%)	7 (7%)	1	1
1	D	82/132 (62%)	60 (73%)	19 (23%)	3 (4%)	2	3
All	All	377/528 (71%)	304 (81%)	57 (15%)	16 (4%)	2	3

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	44	GLU
1	C	102	ILE
1	B	28	VAL

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Mol	Chain	Res	Type
1	C	70	GLU
1	D	47	GLU
1	B	85	GLY
1	C	6	LYS
1	C	100	ASP
1	B	84	ILE
1	C	103	ILE
1	B	110	LYS
1	C	106	LEU
1	C	108	ALA
1	D	5	PRO
1	B	32	ILE
1	D	31	ILE

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	88/110 (80%)	75 (85%)	13 (15%)	3	6
1	B	86/110 (78%)	72 (84%)	14 (16%)	2	4
1	C	92/110 (84%)	83 (90%)	9 (10%)	7	17
1	D	78/110 (71%)	59 (76%)	19 (24%)	1	1
All	All	344/440 (78%)	289 (84%)	55 (16%)	2	4

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	36	LYS
1	A	50	LEU
1	A	52	THR
1	A	58	GLU
1	A	59	GLN
1	A	69	ASP
1	A	77	LYS

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Mol	Chain	Res	Type
1	A	81	LEU
1	A	83	GLU
1	A	90	ARG
1	A	91	LEU
1	A	103	ILE
1	B	7	GLU
1	B	10	ARG
1	B	16	ILE
1	B	21	LEU
1	B	22	LYS
1	B	45	LEU
1	B	47	GLU
1	B	50	LEU
1	B	55	ASP
1	B	56	ARG
1	B	62	ILE
1	B	63	ILE
1	B	81	LEU
1	B	111	LYS
1	C	33	LYS
1	C	34	GLN
1	C	36	LYS
1	C	52	THR
1	C	56	ARG
1	C	69	ASP
1	C	75	ARG
1	C	81	LEU
1	C	107	GLU
1	D	4	ILE
1	D	6	LYS
1	D	16	ILE
1	D	19	ASN
1	D	20	VAL
1	D	32	ILE
1	D	34	GLN
1	D	36	LYS
1	D	39	SER
1	D	43	MET
1	D	44	GLU
1	D	47	GLU
1	D	49	THR
1	D	55	ASP

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Mol	Chain	Res	Type
1	D	57	LEU
1	D	80	ARG
1	D	87	GLU
1	D	101	LYS
1	D	109	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	19	ASN
1	B	14	ASN
1	B	46	ASN
1	B	59	GLN
1	C	19	ASN
1	C	34	GLN
1	D	19	ASN
1	D	34	GLN
1	D	86	HIS
1	D	105	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	8TF	C	201	-	32,38,38	2.95	13 (40%)	44,60,60	1.76	10 (22%)
3	8TF	A	203	-	32,38,38	3.38	14 (43%)	44,60,60	2.79	18 (40%)

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	8TF	C	201	-	-	1/8/68/68	0/5/5/5
3	8TF	A	203	-	-	3/8/68/68	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	203	8TF	CBC-CAX	-9.65	1.38	1.51
3	C	201	8TF	CAK-CAF	-8.31	1.40	1.51
3	A	203	8TF	CBC-CAT	-7.60	1.41	1.53
3	A	203	8TF	CAK-CAF	-7.48	1.41	1.51
3	C	201	8TF	CBC-CAT	-6.90	1.42	1.53
3	C	201	8TF	CBC-CAX	-6.20	1.43	1.51
3	A	203	8TF	CAD-NAA	5.35	1.63	1.48
3	A	203	8TF	CAO-CAN	5.17	1.38	1.33
3	C	201	8TF	CAK-CAN	-4.48	1.46	1.53
3	A	203	8TF	CAK-CAN	-3.90	1.47	1.53
3	A	203	8TF	CAY-CAX	-3.71	1.34	1.39
3	A	203	8TF	CAW-CAX	-3.71	1.35	1.39
3	C	201	8TF	CAD-NAA	3.57	1.58	1.48
3	C	201	8TF	CAG-CAF	-3.57	1.34	1.39
3	C	201	8TF	CAO-CAN	3.47	1.36	1.33
3	A	203	8TF	CAM-CAK	-3.35	1.48	1.54
3	C	201	8TF	CAW-NAB	-3.19	1.33	1.39
3	C	201	8TF	CAE-CAF	-3.09	1.35	1.39
3	C	201	8TF	CAJ-CAE	-2.82	1.35	1.39
3	C	201	8TF	CAY-CAX	-2.78	1.35	1.39
3	A	203	8TF	CAW-NAB	-2.78	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	201	8TF	CBB-CAW	-2.51	1.35	1.39
3	A	203	8TF	CAS-CAT	2.51	1.35	1.33
3	A	203	8TF	CBB-CAW	-2.50	1.35	1.39
3	A	203	8TF	OBG-CAQ	2.47	1.25	1.21
3	C	201	8TF	CAW-CAX	-2.32	1.36	1.39
3	A	203	8TF	CAU-NAB	2.25	1.54	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	203	8TF	CAM-CAK-CAL	-7.41	100.62	111.15
3	A	203	8TF	CAF-CAK-CAN	6.37	106.26	101.37
3	A	203	8TF	CAL-CAK-CAN	5.65	120.09	111.32
3	A	203	8TF	CAJ-CAE-CAF	-5.45	116.49	121.76
3	C	201	8TF	CAM-CAK-CAL	-5.10	103.91	111.15
3	C	201	8TF	CAM-CAK-CAN	5.05	119.16	111.32
3	A	203	8TF	CAD-NAA-CAN	4.97	135.15	125.21
3	A	203	8TF	CAM-CAK-CAF	-4.47	103.83	110.55
3	A	203	8TF	CAX-CBC-CAT	4.31	104.68	101.37
3	A	203	8TF	CAE-NAA-CAN	-3.94	107.21	111.22
3	C	201	8TF	CAE-NAA-CAN	-3.47	107.69	111.22
3	A	203	8TF	CAD-NAA-CAE	-3.46	117.23	124.49
3	A	203	8TF	CAG-CAF-CAE	3.33	123.04	120.01
3	C	201	8TF	CAF-CAK-CAN	3.09	103.74	101.37
3	A	203	8TF	CAK-CAF-CAE	-3.08	106.82	109.61
3	A	203	8TF	CAL-CAK-CAF	3.00	115.06	110.55
3	A	203	8TF	CAW-NAB-CAT	-2.87	108.30	111.22
3	A	203	8TF	CAU-NAB-CAT	2.74	130.69	125.21
3	A	203	8TF	CAI-CAH-CAG	-2.62	117.01	120.24
3	C	201	8TF	CBC-CAT-NAB	2.59	111.01	108.50
3	A	203	8TF	CAF-CAE-NAA	2.55	111.44	109.78
3	C	201	8TF	CBE-CBC-CBD	-2.55	107.52	111.15
3	C	201	8TF	CAJ-CAE-CAF	-2.42	119.42	121.76
3	A	203	8TF	CBD-CBC-CAX	-2.39	106.96	110.55
3	C	201	8TF	CBD-CBC-CAT	2.29	114.87	111.32
3	C	201	8TF	CAX-CAW-NAB	-2.22	108.34	109.78
3	C	201	8TF	CAW-NAB-CAT	-2.05	109.13	111.22
3	A	203	8TF	CAI-CAJ-CAE	2.05	122.42	118.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	203	8TF	CAC-CAD-NAA-CAE
3	A	203	8TF	CAC-CAD-NAA-CAN
3	C	201	8TF	CAC-CAD-NAA-CAE
3	A	203	8TF	CAV-CAU-NAB-CAW

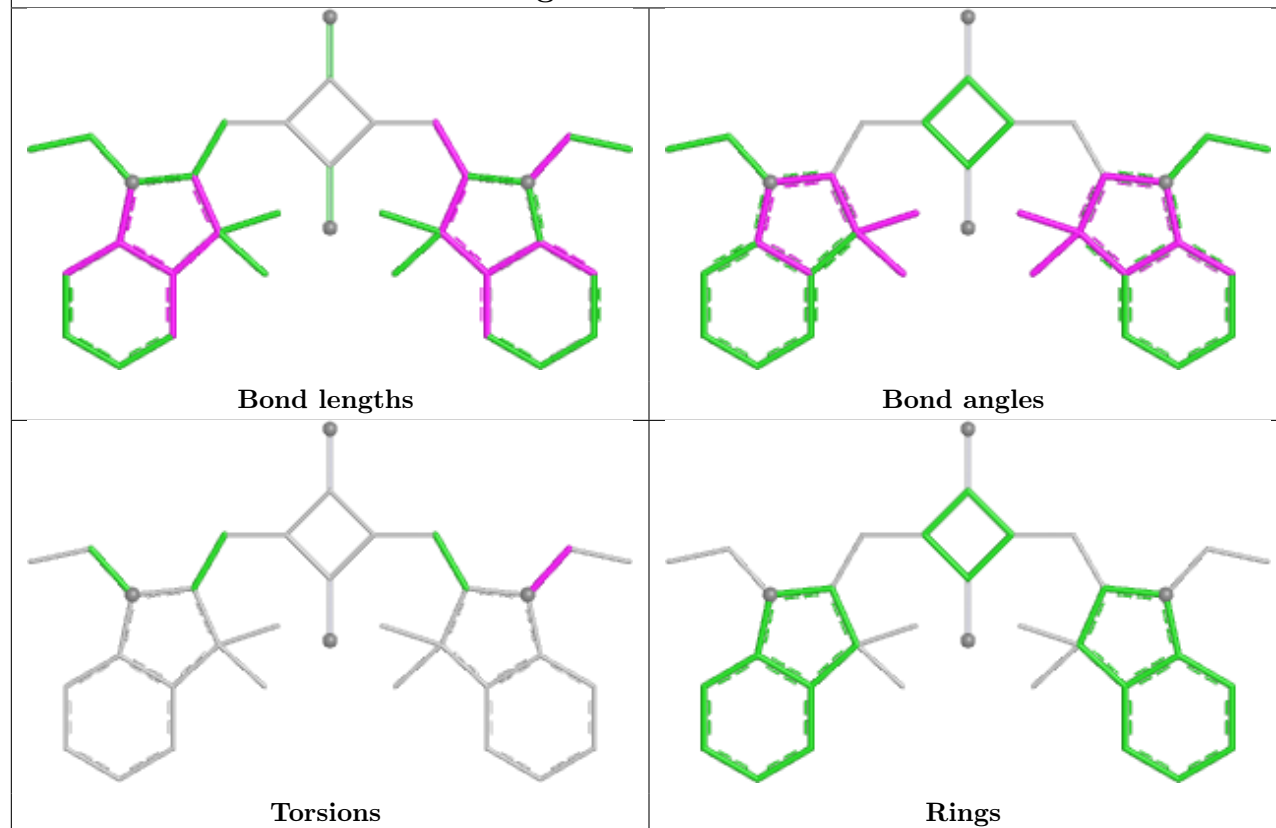
There are no ring outliers.

2 monomers are involved in 8 short contacts:

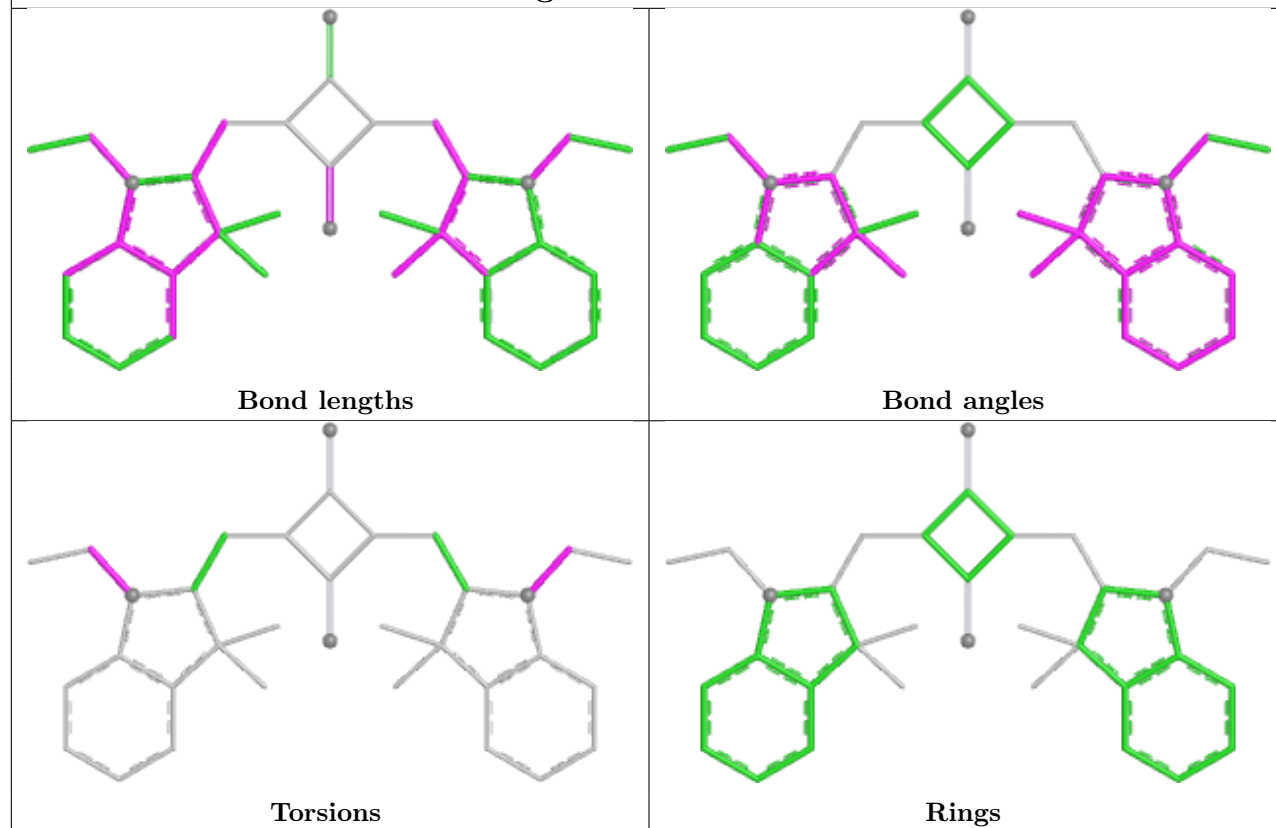
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	201	8TF	3	0
3	A	203	8TF	5	0

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 8TF C 201



Ligand 8TF A 203



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	101/132 (76%)	0.24	2 (1%) 65 60	48, 76, 118, 133	0
1	B	98/132 (74%)	0.64	7 (7%) 22 17	70, 103, 129, 147	0
1	C	105/132 (79%)	0.21	3 (2%) 53 48	39, 72, 119, 127	1 (0%)
1	D	88/132 (66%)	0.60	7 (7%) 18 14	64, 103, 135, 161	0
All	All	392/528 (74%)	0.41	19 (4%) 35 30	39, 90, 129, 161	1 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	54	PHE	4.1
1	B	50	LEU	3.6
1	C	43	MET	3.6
1	B	78	TYR	3.3
1	B	79	TYR	3.2
1	B	53	ILE	3.1
1	D	8	MET	2.9
1	A	48	ALA	2.7
1	D	21	LEU	2.7
1	D	43	MET	2.6
1	D	30	GLY	2.5
1	D	32	ILE	2.4
1	D	31	ILE	2.4
1	C	72	GLN	2.2
1	A	17	LEU	2.1
1	B	43	MET	2.1
1	D	20	VAL	2.1
1	B	67	ALA	2.1
1	C	17	LEU	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](#)

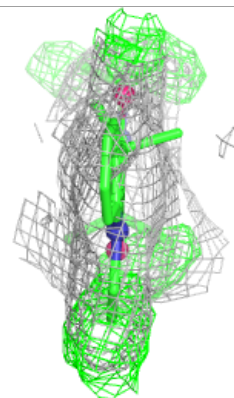
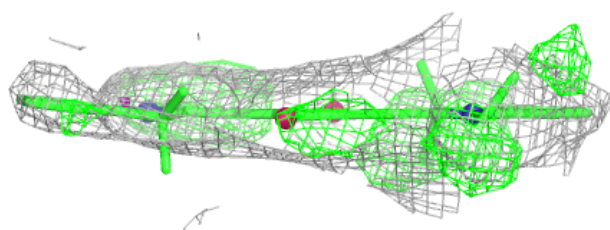
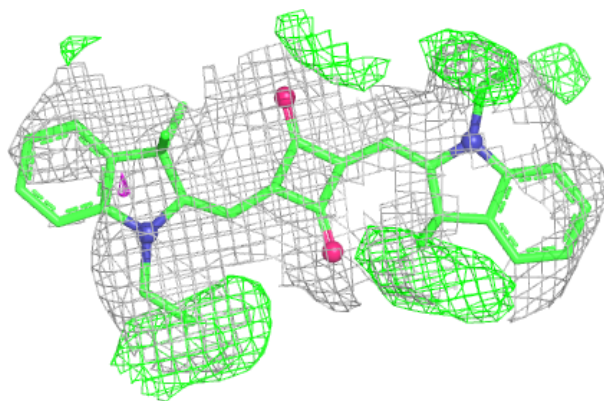
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	8TF	A	203	34/34	0.79	0.21	81,118,148,149	0
3	8TF	C	201	34/34	0.81	0.23	104,123,154,155	0
2	NI	B	202	1/1	0.97	0.05	92,92,92,92	0
2	NI	A	202	1/1	0.97	0.04	83,83,83,83	0
2	NI	B	201	1/1	0.97	0.04	89,89,89,89	0
2	NI	A	201	1/1	0.99	0.03	91,91,91,91	0

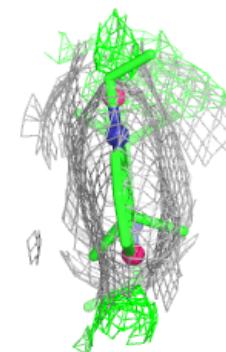
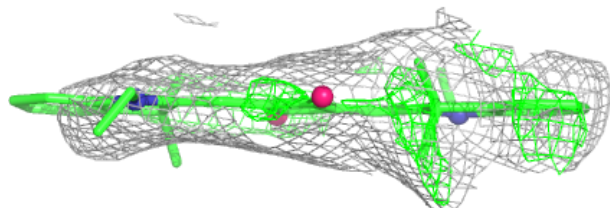
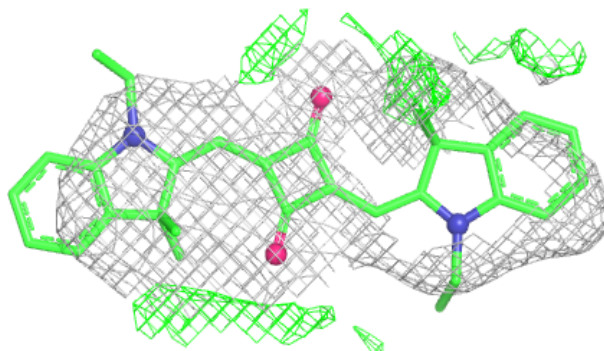
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8TF A 203:

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

**Electron density around 8TF C 201:**

$2mF_o-DF_c$ (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.