



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:10 AM UTC

PDB ID : 6BRM / pdb_00006brm
Title : The crystal structure of isothiocyanate hydrolase from *Delia radicum* gut bacteria
Authors : Tan, K.; van den Bosch, T.; Joachimiak, A.; Welte, C.
Deposited on : 2017-11-30
Resolution : 2.55 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
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

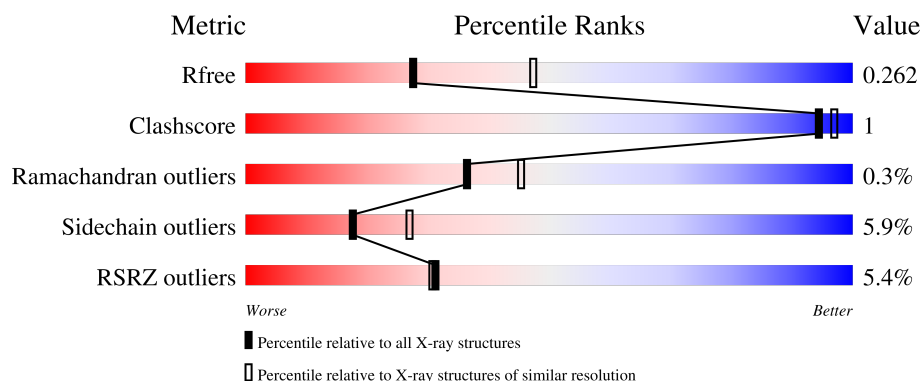
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	269	5% 91% 7%
1	B	269	4% 90% 7%
1	C	269	5% 88% 9%
1	D	269	3% 89% 7%
1	E	269	3% 88% 8%

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Mol	Chain	Length	Quality of chain
1	F	269	6% 88% 8%
1	G	269	6% 88% 9%
1	H	269	10% 88% 7% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16403 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 Putative metal-dependent isothiocyanate hydrolase SaxA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2054	1311	346	387	10			
1	B	263	Total	C	N	O	S	0	1	0
			2073	1325	348	390	10			
1	C	262	Total	C	N	O	S	0	0	0
			2054	1311	346	387	10			
1	D	261	Total	C	N	O	S	0	0	0
			2037	1301	342	384	10			
1	E	261	Total	C	N	O	S	0	0	0
			2049	1308	345	386	10			
1	F	261	Total	C	N	O	S	0	0	0
			2035	1299	340	386	10			
1	G	261	Total	C	N	O	S	0	0	0
			2041	1305	342	384	10			
1	H	256	Total	C	N	O	S	0	0	0
			1990	1271	332	377	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	SER	-	expression tag	UNP A0A0N7FW12
A	261	ALA	-	expression tag	UNP A0A0N7FW12
A	262	TRP	-	expression tag	UNP A0A0N7FW12
A	263	SER	-	expression tag	UNP A0A0N7FW12
A	264	HIS	-	expression tag	UNP A0A0N7FW12
A	265	PRO	-	expression tag	UNP A0A0N7FW12
A	266	GLN	-	expression tag	UNP A0A0N7FW12
A	267	PHE	-	expression tag	UNP A0A0N7FW12
A	268	GLU	-	expression tag	UNP A0A0N7FW12
A	269	LYS	-	expression tag	UNP A0A0N7FW12
B	260	SER	-	expression tag	UNP A0A0N7FW12
B	261	ALA	-	expression tag	UNP A0A0N7FW12
B	262	TRP	-	expression tag	UNP A0A0N7FW12

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Chain	Residue	Modelled	Actual	Comment	Reference
B	263	SER	-	expression tag	UNP A0A0N7FW12
B	264	HIS	-	expression tag	UNP A0A0N7FW12
B	265	PRO	-	expression tag	UNP A0A0N7FW12
B	266	GLN	-	expression tag	UNP A0A0N7FW12
B	267	PHE	-	expression tag	UNP A0A0N7FW12
B	268	GLU	-	expression tag	UNP A0A0N7FW12
B	269	LYS	-	expression tag	UNP A0A0N7FW12
C	260	SER	-	expression tag	UNP A0A0N7FW12
C	261	ALA	-	expression tag	UNP A0A0N7FW12
C	262	TRP	-	expression tag	UNP A0A0N7FW12
C	263	SER	-	expression tag	UNP A0A0N7FW12
C	264	HIS	-	expression tag	UNP A0A0N7FW12
C	265	PRO	-	expression tag	UNP A0A0N7FW12
C	266	GLN	-	expression tag	UNP A0A0N7FW12
C	267	PHE	-	expression tag	UNP A0A0N7FW12
C	268	GLU	-	expression tag	UNP A0A0N7FW12
C	269	LYS	-	expression tag	UNP A0A0N7FW12
D	260	SER	-	expression tag	UNP A0A0N7FW12
D	261	ALA	-	expression tag	UNP A0A0N7FW12
D	262	TRP	-	expression tag	UNP A0A0N7FW12
D	263	SER	-	expression tag	UNP A0A0N7FW12
D	264	HIS	-	expression tag	UNP A0A0N7FW12
D	265	PRO	-	expression tag	UNP A0A0N7FW12
D	266	GLN	-	expression tag	UNP A0A0N7FW12
D	267	PHE	-	expression tag	UNP A0A0N7FW12
D	268	GLU	-	expression tag	UNP A0A0N7FW12
D	269	LYS	-	expression tag	UNP A0A0N7FW12
E	260	SER	-	expression tag	UNP A0A0N7FW12
E	261	ALA	-	expression tag	UNP A0A0N7FW12
E	262	TRP	-	expression tag	UNP A0A0N7FW12
E	263	SER	-	expression tag	UNP A0A0N7FW12
E	264	HIS	-	expression tag	UNP A0A0N7FW12
E	265	PRO	-	expression tag	UNP A0A0N7FW12
E	266	GLN	-	expression tag	UNP A0A0N7FW12
E	267	PHE	-	expression tag	UNP A0A0N7FW12
E	268	GLU	-	expression tag	UNP A0A0N7FW12
E	269	LYS	-	expression tag	UNP A0A0N7FW12
F	260	SER	-	expression tag	UNP A0A0N7FW12
F	261	ALA	-	expression tag	UNP A0A0N7FW12
F	262	TRP	-	expression tag	UNP A0A0N7FW12
F	263	SER	-	expression tag	UNP A0A0N7FW12
F	264	HIS	-	expression tag	UNP A0A0N7FW12

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Chain	Residue	Modelled	Actual	Comment	Reference
F	265	PRO	-	expression tag	UNP A0A0N7FW12
F	266	GLN	-	expression tag	UNP A0A0N7FW12
F	267	PHE	-	expression tag	UNP A0A0N7FW12
F	268	GLU	-	expression tag	UNP A0A0N7FW12
F	269	LYS	-	expression tag	UNP A0A0N7FW12
G	260	SER	-	expression tag	UNP A0A0N7FW12
G	261	ALA	-	expression tag	UNP A0A0N7FW12
G	262	TRP	-	expression tag	UNP A0A0N7FW12
G	263	SER	-	expression tag	UNP A0A0N7FW12
G	264	HIS	-	expression tag	UNP A0A0N7FW12
G	265	PRO	-	expression tag	UNP A0A0N7FW12
G	266	GLN	-	expression tag	UNP A0A0N7FW12
G	267	PHE	-	expression tag	UNP A0A0N7FW12
G	268	GLU	-	expression tag	UNP A0A0N7FW12
G	269	LYS	-	expression tag	UNP A0A0N7FW12
H	260	SER	-	expression tag	UNP A0A0N7FW12
H	261	ALA	-	expression tag	UNP A0A0N7FW12
H	262	TRP	-	expression tag	UNP A0A0N7FW12
H	263	SER	-	expression tag	UNP A0A0N7FW12
H	264	HIS	-	expression tag	UNP A0A0N7FW12
H	265	PRO	-	expression tag	UNP A0A0N7FW12
H	266	GLN	-	expression tag	UNP A0A0N7FW12
H	267	PHE	-	expression tag	UNP A0A0N7FW12
H	268	GLU	-	expression tag	UNP A0A0N7FW12
H	269	LYS	-	expression tag	UNP A0A0N7FW12

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

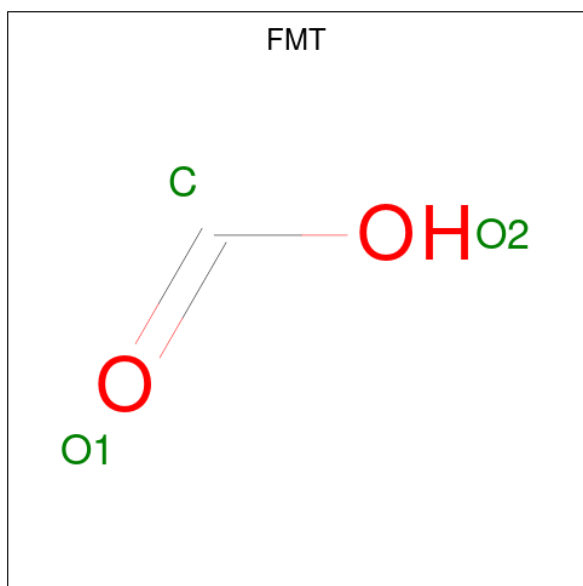
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0
2	E	2	Total Zn 2 2	0	0
2	F	2	Total Zn 2 2	0	0
2	G	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	2	Total	Zn	0	0
			2	2		

- Molecule 3 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	C	1	Total	C	O	0	0
			3	1	2		
3	E	1	Total	C	O	0	0
			3	1	2		
3	G	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	7	Total	O	0	0
			7	7		
4	C	6	Total	O	0	0
			6	6		
4	D	5	Total	O	0	0
			5	5		

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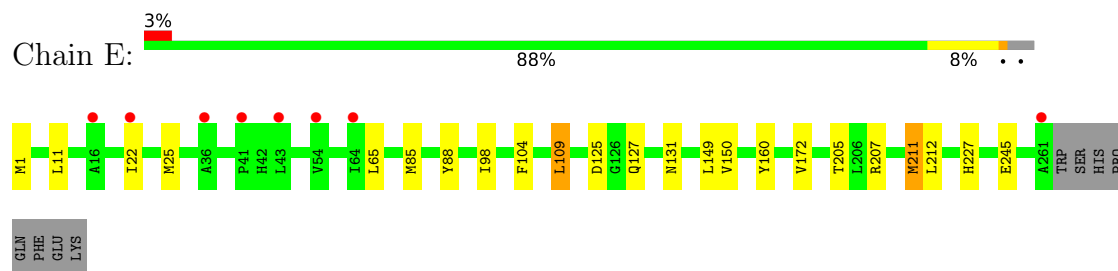
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	5	Total 5	O 5	0	0
4	F	5	Total 5	O 5	0	0
4	G	5	Total 5	O 5	0	0
4	H	4	Total 4	O 4	0	0

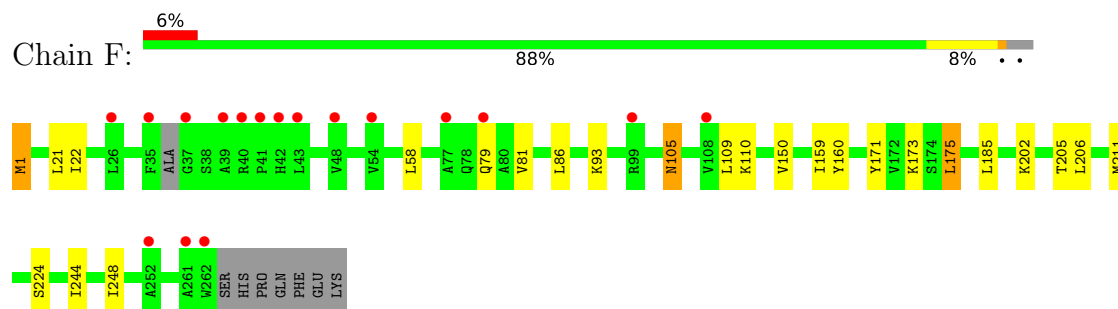
- Molecule 1: Putative metal-dependent isothiocyanate hydrolase SaxA



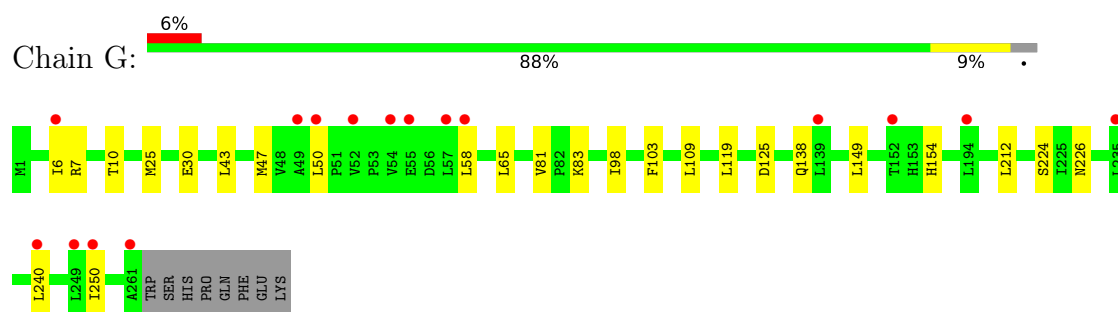
- Molecule 1: Putative metal-dependent isothiocyanate hydrolase SaxA



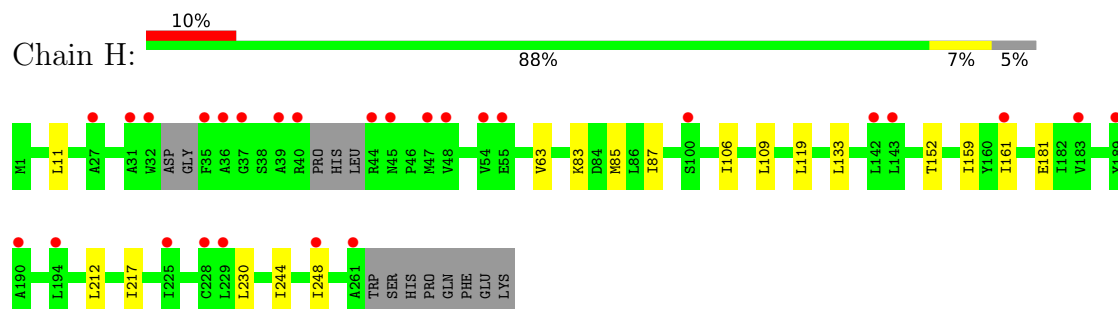
- Molecule 1: Putative metal-dependent isothiocyanate hydrolase SaxA



- Molecule 1: Putative metal-dependent isothiocyanate hydrolase SaxA



- Molecule 1: Putative metal-dependent isothiocyanate hydrolase SaxA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	179.16Å 79.53Å 90.41Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	49.84 – 2.55 49.84 – 2.55	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.84-2.55) 98.5 (49.84-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.206 , 0.243 0.221 , 0.262	Depositor DCC
R_{free} test set	4116 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.226	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 14.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
Reported twinning fraction	0.657 for H, K, L 0.343 for -h,-k,l	Depositor
Outliers	5 of 82280 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16403	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 73.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7105e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FMT

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	0.54	0/2098	0.76	2/2850 (0.1%)
1	B	0.55	0/2118	0.75	0/2877
1	C	0.55	0/2098	0.74	0/2850
1	D	0.55	0/2081	0.79	0/2828
1	E	0.54	0/2093	0.76	0/2843
1	F	0.52	0/2077	0.74	0/2821
1	G	0.56	0/2085	0.77	0/2833
1	H	0.54	0/2029	0.76	0/2755
All	All	0.54	0/16679	0.76	2/22657 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	LEU	CA-C-N	5.19	125.24	119.32
1	A	212	LEU	C-N-CA	5.19	125.24	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2054	0	2044	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2073	0	2060	3	0
1	C	2054	0	2044	6	0
1	D	2037	0	2020	7	0
1	E	2049	0	2042	5	0
1	F	2035	0	2013	9	0
1	G	2041	0	2031	9	0
1	H	1990	0	1975	3	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	3	0	1	0	0
3	C	3	0	1	0	0
3	E	3	0	1	0	0
3	G	3	0	1	0	0
4	A	5	0	0	0	0
4	B	7	0	0	0	0
4	C	6	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	4	0	0	0	0
All	All	16403	0	16233	43	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 1.

All (43) 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:218:VAL:HG13	1:B:257:MET:HE1	1.83	0.60
1:C:185:LEU:HD22	1:C:200:MET:HE1	1.83	0.60
1:G:43:LEU:HD13	1:G:47:MET:HE2	1.84	0.60
1:H:244:ILE:HD12	1:H:248:ILE:HD11	1.89	0.54
1:G:6:ILE:HB	1:G:10:THR:HG23	1.91	0.53
1:D:192:ASN:HB2	1:D:198:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:65:LEU:HD12	1:G:98:ILE:HD11	1.90	0.53
1:B:153:HIS:ND1	1:B:154:HIS:O	2.24	0.53
1:F:244:ILE:HD12	1:F:248:ILE:HD11	1.91	0.52
1:F:171:TYR:CZ	1:F:175:LEU:HD21	2.48	0.48
1:F:58:LEU:HD22	1:F:81:VAL:HG12	1.96	0.48
1:G:7:ARG:O	1:G:10:THR:HG22	2.13	0.48
1:C:185:LEU:HD13	1:C:200:MET:CE	2.44	0.46
1:F:22:ILE:HD12	1:F:22:ILE:N	2.31	0.46
1:A:240:LEU:HD23	1:A:245:GLU:HG2	1.97	0.46
1:F:105:ASN:HD21	1:G:154:HIS:HB2	1.81	0.46
1:B:1:MET:HE1	1:B:159:ILE:HD12	1.97	0.45
1:C:150:VAL:HG22	1:C:160:TYR:CD1	2.52	0.45
1:C:222:MET:HE1	1:C:235:LEU:HD22	1.98	0.45
1:D:127:GLN:HB3	1:D:168:VAL:HG21	1.97	0.45
1:D:7:ARG:O	1:D:10:THR:HG22	2.16	0.45
1:A:218:VAL:HG22	1:A:257:MET:HE1	1.99	0.45
1:F:205:THR:HG21	1:F:248:ILE:HG12	1.99	0.45
1:H:87:ILE:HB	1:H:106:ILE:HG22	1.98	0.45
1:E:172:VAL:HG13	1:E:211:MET:HE2	1.97	0.45
1:F:150:VAL:HG22	1:F:160:TYR:CD1	2.52	0.44
1:D:164:ASP:OD1	1:D:186:ASN:ND2	2.44	0.43
1:G:98:ILE:HG22	1:G:103:PHE:HB2	1.99	0.43
1:E:150:VAL:HG22	1:E:160:TYR:CD1	2.53	0.43
1:G:47:MET:HE3	1:G:226:ASN:HA	2.01	0.43
1:E:127:GLN:HE22	1:E:131:ASN:ND2	2.16	0.43
1:D:205:THR:CG2	1:D:248:ILE:HD12	2.48	0.43
1:A:116:VAL:HG11	1:D:119:LEU:HD12	2.02	0.42
1:F:105:ASN:HD21	1:G:154:HIS:CB	2.31	0.42
1:A:217:ILE:HD12	1:A:217:ILE:N	2.35	0.42
1:G:58:LEU:HD21	1:G:81:VAL:HG22	2.01	0.42
1:H:244:ILE:HD12	1:H:248:ILE:CD1	2.49	0.42
1:E:65:LEU:HD12	1:E:98:ILE:HD13	2.00	0.42
1:C:1:MET:HE1	1:C:159:ILE:HD12	2.01	0.42
1:F:1:MET:HE1	1:F:159:ILE:HB	2.02	0.41
1:D:45:ASN:HA	1:D:46:PRO:C	2.45	0.41
1:E:88:TYR:HB3	1:E:109:LEU:HD13	2.04	0.40
1:C:235:LEU:HD23	1:C:250:ILE:HD12	2.04	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	260/269 (97%)	242 (93%)	17 (6%)	1 (0%)	30	39
1	B	262/269 (97%)	244 (93%)	16 (6%)	2 (1%)	16	22
1	C	260/269 (97%)	250 (96%)	9 (4%)	1 (0%)	30	39
1	D	259/269 (96%)	241 (93%)	18 (7%)	0	100	100
1	E	259/269 (96%)	246 (95%)	13 (5%)	0	100	100
1	F	257/269 (96%)	239 (93%)	17 (7%)	1 (0%)	30	39
1	G	259/269 (96%)	241 (93%)	17 (7%)	1 (0%)	30	39
1	H	250/269 (93%)	232 (93%)	18 (7%)	0	100	100
All	All	2066/2152 (96%)	1935 (94%)	125 (6%)	6 (0%)	36	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	224	SER
1	A	224	SER
1	C	194	LEU
1	F	224	SER
1	B	73	TRP
1	B	37	GLY

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	220/228 (96%)	210 (96%)	10 (4%)	24	38
1	B	222/228 (97%)	209 (94%)	13 (6%)	18	27
1	C	220/228 (96%)	204 (93%)	16 (7%)	13	18
1	D	217/228 (95%)	208 (96%)	9 (4%)	27	41
1	E	220/228 (96%)	205 (93%)	15 (7%)	14	20
1	F	217/228 (95%)	203 (94%)	14 (6%)	15	22
1	G	218/228 (96%)	206 (94%)	12 (6%)	19	29
1	H	212/228 (93%)	198 (93%)	14 (7%)	15	21
All	All	1746/1824 (96%)	1643 (94%)	103 (6%)	18	27

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	65	LEU
1	A	97	LEU
1	A	109	LEU
1	A	149	LEU
1	A	156	GLU
1	A	177	ARG
1	A	194	LEU
1	A	210	LYS
1	A	227	HIS
1	B	3	LEU
1	B	7	ARG
1	B	11	LEU
1	B	60	VAL
1	B	65	LEU
1	B	109	LEU
1	B	142	LEU
1	B	152	THR
1	B	169	LYS
1	B	211	MET
1	B	230	LEU
1	B	232	ARG
1	B	257	MET
1	C	5	GLN
1	C	21	LEU
1	C	45	ASN
1	C	57	LEU

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Mol	Chain	Res	Type
1	C	64	ILE
1	C	93	LYS
1	C	119	LEU
1	C	125	ASP
1	C	136	ASP
1	C	152	THR
1	C	173	LYS
1	C	177	ARG
1	C	194	LEU
1	C	211	MET
1	C	217	ILE
1	C	230	LEU
1	D	21	LEU
1	D	42	HIS
1	D	57	LEU
1	D	139	LEU
1	D	149	LEU
1	D	156	GLU
1	D	191	VAL
1	D	198	ILE
1	D	203	GLU
1	E	1	MET
1	E	11	LEU
1	E	22	ILE
1	E	25	MET
1	E	85	MET
1	E	104	PHE
1	E	109	LEU
1	E	125	ASP
1	E	149	LEU
1	E	205	THR
1	E	207	ARG
1	E	211	MET
1	E	212	LEU
1	E	227	HIS
1	E	245	GLU
1	F	1	MET
1	F	21	LEU
1	F	79	GLN
1	F	86	LEU
1	F	93	LYS
1	F	105	ASN

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Mol	Chain	Res	Type
1	F	109	LEU
1	F	110	LYS
1	F	173	LYS
1	F	175	LEU
1	F	185	LEU
1	F	202	LYS
1	F	206	LEU
1	F	211	MET
1	G	25	MET
1	G	30	GLU
1	G	50	LEU
1	G	83	LYS
1	G	109	LEU
1	G	119	LEU
1	G	125	ASP
1	G	138	GLN
1	G	149	LEU
1	G	212	LEU
1	G	240	LEU
1	G	250	ILE
1	H	11	LEU
1	H	63	VAL
1	H	83	LYS
1	H	85	MET
1	H	109	LEU
1	H	119	LEU
1	H	133	LEU
1	H	152	THR
1	H	159	ILE
1	H	161	ILE
1	H	181	GLU
1	H	212	LEU
1	H	217	ILE
1	H	230	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	90	GLN
1	A	138	GLN
1	A	154	HIS

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Mol	Chain	Res	Type
1	B	14	GLN
1	B	101	GLN
1	C	78	GLN
1	C	131	ASN
1	D	8	ASN
1	E	5	GLN
1	E	14	GLN
1	E	78	GLN
1	E	131	ASN
1	E	176	GLN
1	F	8	ASN
1	F	90	GLN
1	F	192	ASN
1	G	113	ASN
1	G	127	GLN
1	G	153	HIS
1	H	14	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FMT	A	303	-	2,2,2	0.71	0	1,1,1	0.70	0
3	FMT	G	303	-	2,2,2	0.68	0	1,1,1	0.70	0
3	FMT	C	303	-	2,2,2	0.67	0	1,1,1	0.71	0
3	FMT	E	303	-	2,2,2	0.69	0	1,1,1	0.70	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	262/269 (97%)	0.51	13 (4%) 34 33	39, 56, 69, 86	0
1	B	263/269 (97%)	0.60	10 (3%) 44 45	30, 56, 77, 101	1 (0%)
1	C	262/269 (97%)	0.56	13 (4%) 34 33	36, 55, 85, 114	0
1	D	261/269 (97%)	0.49	8 (3%) 51 52	37, 52, 72, 96	0
1	E	261/269 (97%)	0.53	8 (3%) 51 52	39, 56, 83, 105	0
1	F	261/269 (97%)	0.70	17 (6%) 25 24	37, 58, 83, 111	0
1	G	261/269 (97%)	0.67	16 (6%) 27 26	45, 62, 77, 91	0
1	H	256/269 (95%)	1.02	27 (10%) 11 11	43, 67, 87, 98	0
All	All	2087/2152 (96%)	0.64	112 (5%) 31 31	30, 58, 82, 114	1 (0%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	37	GLY	6.2
1	F	262	TRP	5.9
1	H	40	ARG	5.3
1	G	261	ALA	4.8
1	H	229	LEU	4.7
1	F	39	ALA	4.6
1	G	55	GLU	4.5
1	E	43	LEU	4.5
1	B	27	ALA	4.5
1	H	44	ARG	4.3
1	F	261	ALA	4.2
1	D	261	ALA	4.2
1	H	35	PHE	4.1
1	C	262	TRP	4.1
1	F	40	ARG	4.1
1	A	262	TRP	4.0

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Mol	Chain	Res	Type	RSRZ
1	H	183	VAL	3.9
1	F	41	PRO	3.6
1	H	39	ALA	3.3
1	F	77	ALA	3.3
1	F	42	HIS	3.2
1	E	261	ALA	3.2
1	H	32	TRP	3.2
1	C	42	HIS	3.2
1	C	43	LEU	3.2
1	D	43	LEU	3.1
1	H	36	ALA	3.1
1	B	26	LEU	3.1
1	F	43	LEU	3.1
1	F	54	VAL	3.1
1	G	250	ILE	3.1
1	C	36	ALA	3.0
1	F	37	GLY	3.0
1	E	36	ALA	3.0
1	B	36	ALA	2.9
1	B	262	TRP	2.9
1	G	49	ALA	2.9
1	B	42	HIS	2.8
1	C	194	LEU	2.8
1	H	48	VAL	2.8
1	H	225	ILE	2.8
1	F	35	PHE	2.8
1	A	58	LEU	2.8
1	H	248	ILE	2.7
1	F	26	LEU	2.7
1	D	42	HIS	2.7
1	G	6	ILE	2.7
1	C	41	PRO	2.6
1	H	190	ALA	2.6
1	C	37	GLY	2.6
1	C	208	THR	2.6
1	A	55	GLU	2.5
1	H	55	GLU	2.5
1	F	48	VAL	2.5
1	C	261	ALA	2.5
1	H	27	ALA	2.5
1	F	99	ARG	2.5
1	B	41	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	54	VAL	2.5
1	H	100	SER	2.5
1	F	79	GLN	2.5
1	D	39	ALA	2.5
1	E	16	ALA	2.5
1	G	58	LEU	2.4
1	H	143	LEU	2.4
1	D	98	ILE	2.4
1	A	248	ILE	2.4
1	A	97	LEU	2.4
1	G	235	LEU	2.4
1	E	64	ILE	2.3
1	D	154	HIS	2.3
1	H	142	LEU	2.3
1	H	228	CYS	2.3
1	F	108	VAL	2.3
1	G	50	LEU	2.3
1	H	47	MET	2.3
1	E	54	VAL	2.3
1	H	45	ASN	2.3
1	A	62	ALA	2.3
1	A	52	VAL	2.3
1	D	37	GLY	2.3
1	A	57	LEU	2.3
1	B	1	MET	2.2
1	C	260	SER	2.2
1	A	20	PHE	2.2
1	G	54	VAL	2.2
1	G	139	LEU	2.2
1	G	194	LEU	2.2
1	B	261	ALA	2.2
1	G	152	THR	2.2
1	D	41	PRO	2.2
1	B	258	ALA	2.1
1	C	39	ALA	2.1
1	A	65	LEU	2.1
1	B	57	LEU	2.1
1	G	240	LEU	2.1
1	A	32	TRP	2.1
1	G	57	LEU	2.1
1	C	54	VAL	2.1
1	G	52	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	49	ALA	2.1
1	F	252	ALA	2.1
1	H	31	ALA	2.1
1	A	91	ASP	2.1
1	H	189	TYR	2.1
1	E	41	PRO	2.1
1	G	249	LEU	2.0
1	C	64	ILE	2.0
1	H	161	ILE	2.0
1	H	194	LEU	2.0
1	H	261	ALA	2.0
1	E	22	ILE	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
3	FMT	A	303	3/3	0.70	0.21	51,51,54,55	0
3	FMT	G	303	3/3	0.74	0.38	83,83,84,86	0
3	FMT	E	303	3/3	0.80	0.18	64,64,66,67	0
3	FMT	C	303	3/3	0.83	0.18	67,67,68,69	0
2	ZN	D	302	1/1	0.94	0.06	41,41,41,41	0
2	ZN	D	301	1/1	0.98	0.05	38,38,38,38	0
2	ZN	B	301	1/1	0.98	0.04	48,48,48,48	0
2	ZN	F	302	1/1	0.99	0.02	44,44,44,44	0
2	ZN	G	301	1/1	0.99	0.03	52,52,52,52	0
2	ZN	G	302	1/1	0.99	0.02	54,54,54,54	0
2	ZN	H	301	1/1	0.99	0.02	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	H	302	1/1	0.99	0.03	59,59,59,59	0
2	ZN	A	301	1/1	0.99	0.03	45,45,45,45	0
2	ZN	C	302	1/1	0.99	0.03	47,47,47,47	0
2	ZN	E	301	1/1	0.99	0.02	49,49,49,49	0
2	ZN	F	301	1/1	0.99	0.03	52,52,52,52	0
2	ZN	A	302	1/1	1.00	0.01	47,47,47,47	0
2	ZN	E	302	1/1	1.00	0.02	51,51,51,51	0
2	ZN	B	302	1/1	1.00	0.03	52,52,52,52	0
2	ZN	C	301	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.