



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:12 PM UTC

PDB ID : 4M8D / pdb_00004m8d
Title : Crystal structure of an isatin hydrolase bound to product analogue thioisatinate
Authors : Bjerregaard-Andersen, K.; Sommer, T.; Jensen, J.K.; Jochimsen, B.; Etzerodt, M.; Morth, J.P.
Deposited on : 2013-08-13
Resolution : 1.90 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

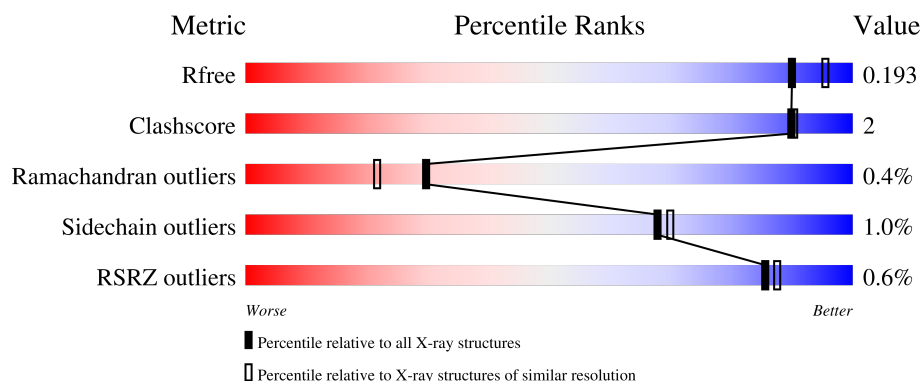
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

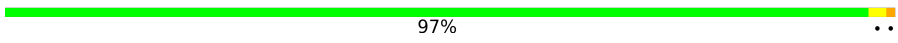
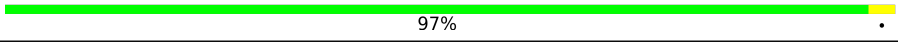
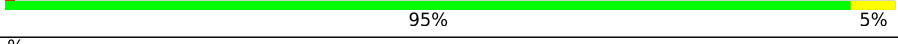
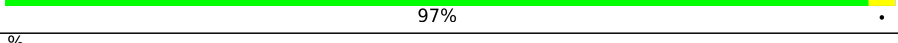
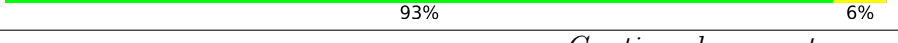
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	263	 97% ..
1	B	263	 97% .
1	C	263	 95% 5%
1	D	263	 97% .
1	E	263	 93% 6%

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Mol	Chain	Length	Quality of chain
1	F	263	% 97%
1	G	263	95% 5%
1	H	263	% 94% 6%
1	I	263	91% 8%
1	J	263	92% 8%
1	K	263	95%
1	L	263	93% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27233 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 uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	1	0
			1978	1257	333	380	8			
1	B	262	Total	C	N	O	S	0	1	0
			1973	1254	332	380	7			
1	C	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	D	263	Total	C	N	O	S	0	0	0
			1978	1257	333	380	8			
1	E	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	F	263	Total	C	N	O	S	0	0	0
			1977	1257	333	379	8			
1	G	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	H	263	Total	C	N	O	S	0	0	0
			1978	1257	333	380	8			
1	I	262	Total	C	N	O	S	0	1	0
			1980	1259	335	378	8			
1	J	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	K	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			
1	L	262	Total	C	N	O	S	0	0	0
			1972	1254	332	378	8			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

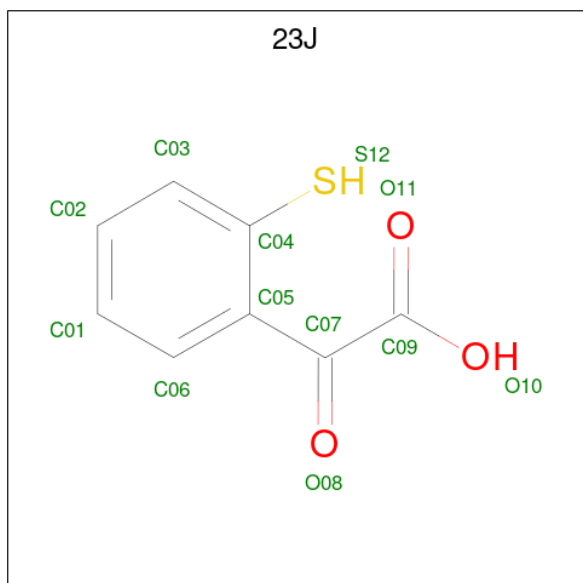
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		
2	G	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	I	1	Total	Mn	0	0
			1	1		
2	J	1	Total	Mn	0	0
			1	1		
2	K	1	Total	Mn	0	0
			1	1		
2	L	1	Total	Mn	0	0
			1	1		

- Molecule 3 is oxo(2-sulfanylphenyl)acetic acid (CCD ID: 23J) (formula: $C_8H_6O_3S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			12	8	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	S	0	1
			24	16	6	2		
3	C	1	Total	C	O	S	0	0
			12	8	3	1		
3	D	1	Total	C	O	S	0	0
			12	8	3	1		
3	E	1	Total	C	O	S	0	0
			12	8	3	1		
3	F	1	Total	C	O	S	0	1
			24	16	6	2		
3	G	1	Total	C	O	S	0	1
			24	16	6	2		
3	H	1	Total	C	O	S	0	0
			12	8	3	1		
3	I	1	Total	C	O	S	0	0
			12	8	3	1		
3	J	1	Total	C	O	S	0	0
			12	8	3	1		
3	K	1	Total	C	O	S	0	0
			12	8	3	1		
3	L	1	Total	C	O	S	0	0
			12	8	3	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Ca	0	0
			3	3		
4	B	3	Total	Ca	0	0
			3	3		
4	C	2	Total	Ca	0	0
			2	2		
4	D	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		
4	I	1	Total	Ca	0	0
			1	1		
4	J	2	Total	Ca	0	0
			2	2		
4	L	3	Total	Ca	0	0
			3	3		

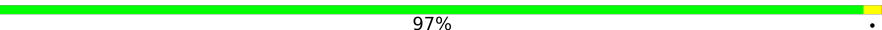
- Molecule 5 is water.

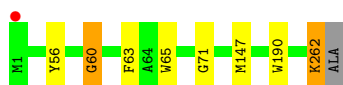
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	318	Total 318	O 318	0	0
5	B	323	Total 323	O 323	0	0
5	C	237	Total 237	O 237	0	0
5	D	293	Total 293	O 293	0	0
5	E	266	Total 266	O 266	0	0
5	F	320	Total 320	O 320	0	0
5	G	240	Total 240	O 240	0	0
5	H	237	Total 237	O 237	0	0
5	I	282	Total 282	O 282	0	0
5	J	259	Total 259	O 259	0	0
5	K	279	Total 279	O 279	0	0
5	L	275	Total 275	O 275	0	0

3 Residue-property plots

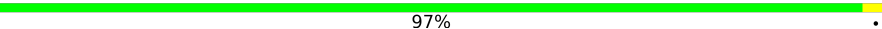
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Putative uncharacterized protein

Chain A:  97% ..

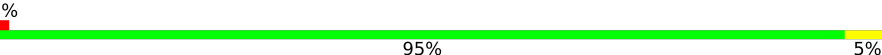


- Molecule 1: Putative uncharacterized protein

Chain B:  97% .

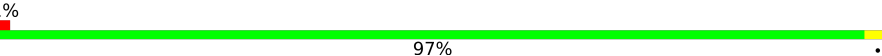


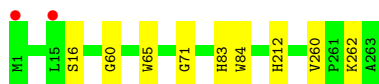
- Molecule 1: Putative uncharacterized protein

Chain C:  95% 5%



- Molecule 1: Putative uncharacterized protein

Chain D:  97% .



- Molecule 1: Putative uncharacterized protein

Chain E:  93% 6%



- Molecule 1: Putative uncharacterized protein



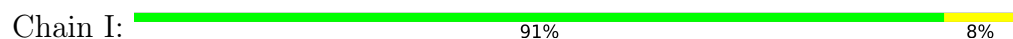
- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



- Molecule 1: Putative uncharacterized protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.98Å 51.82Å 357.09Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	29.98 – 1.90 29.98 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.98-1.90) 97.8 (29.98-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.152 , 0.192 0.154 , 0.193	Depositor DCC
R_{free} test set	14130 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27233	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 26.76 % 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 2.4828e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 23J, MN

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	0.52	0/2032	0.76	2/2772 (0.1%)
1	B	0.50	0/2030	0.75	0/2769
1	C	0.43	0/2026	0.73	0/2764
1	D	0.48	0/2032	0.75	0/2771
1	E	0.48	0/2026	0.76	1/2764 (0.0%)
1	F	0.48	0/2031	0.75	1/2771 (0.0%)
1	G	0.46	0/2026	0.76	2/2764 (0.1%)
1	H	0.44	0/2032	0.73	0/2771
1	I	0.46	0/2037	0.76	0/2778
1	J	0.46	0/2026	0.76	0/2764
1	K	0.47	0/2026	0.75	0/2764
1	L	0.47	0/2026	0.73	2/2764 (0.1%)
All	All	0.47	0/24350	0.75	8/33216 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2	SER	N-CA-C	5.50	117.18	110.41
1	G	168	GLY	CA-C-N	5.35	125.11	119.76
1	G	168	GLY	C-N-CA	5.35	125.11	119.76
1	A	60	GLY	CA-C-N	5.10	125.14	119.32
1	A	60	GLY	C-N-CA	5.10	125.14	119.32
1	L	60	GLY	CA-C-N	5.06	124.67	119.05
1	L	60	GLY	C-N-CA	5.06	124.67	119.05
1	E	53	ILE	N-CA-C	-5.04	106.76	111.45

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	1978	0	1922	5	0
1	B	1973	0	1915	5	0
1	C	1972	0	1918	7	0
1	D	1978	0	1923	5	0
1	E	1972	0	1918	10	0
1	F	1977	0	1923	4	0
1	G	1972	0	1918	6	0
1	H	1978	0	1923	10	0
1	I	1980	0	1931	13	0
1	J	1972	0	1918	14	0
1	K	1972	0	1918	6	0
1	L	1972	0	1918	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	12	0	5	0	0
3	B	24	0	10	3	0
3	C	12	0	5	2	0
3	D	12	0	5	1	0
3	E	12	0	5	1	0
3	F	24	0	10	4	0
3	G	24	0	10	1	0
3	H	12	0	5	1	0
3	I	12	0	5	1	0
3	J	12	0	5	1	0
3	K	12	0	5	2	0
3	L	12	0	5	1	0
4	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	I	1	0	0	0	0
4	J	2	0	0	0	0
4	L	3	0	0	0	0
5	A	318	0	0	1	0
5	B	323	0	0	1	0
5	C	237	0	0	1	0
5	D	293	0	0	0	0
5	E	266	0	0	0	0
5	F	320	0	0	0	0
5	G	240	0	0	0	0
5	H	237	0	0	0	0
5	I	282	0	0	2	0
5	J	259	0	0	0	0
5	K	279	0	0	1	0
5	L	275	0	0	0	0
All	All	27233	0	23120	84	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 2.

All (84) 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:83:HIS:NE2	3:B:302[B]:23J:O10	2.14	0.79
1:A:262:LYS:O	5:A:711:HOH:O	2.12	0.67
1:J:176:PRO:HD3	1:J:205:MET:HE2	1.77	0.67
1:F:83:HIS:NE2	3:F:302[A]:23J:O11	2.31	0.63
1:E:63:PHE:CE1	3:F:302[B]:23J:H1	2.35	0.62
1:C:83:HIS:NE2	3:C:302:23J:O11	2.33	0.61
1:L:1:MET:HE2	1:L:5:SER:HB3	1.83	0.60
1:K:83:HIS:NE2	3:K:302:23J:O10	2.34	0.60
1:G:67:TRP:HA	1:H:71:GLY:HA2	1.84	0.59
1:I:146:VAL:HG13	1:I:229:LEU:HD13	1.85	0.58
1:B:153:LYS:HD2	1:D:16:SER:HB2	1.86	0.58
1:L:83:HIS:NE2	3:L:302:23J:O11	2.36	0.58
1:K:138:GLU:OE1	1:K:185:LYS:NZ	2.32	0.58
3:C:302:23J:O10	5:C:469:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:180:GLU:HG2	1:H:214:LEU:HD13	1.88	0.56
1:I:67:TRP:HA	1:J:71:GLY:HA2	1.88	0.55
1:E:1:MET:N	1:E:2:SER:HA	2.22	0.54
1:K:261:PRO:O	1:K:262:LYS:HB2	2.07	0.54
1:I:261:PRO:O	1:I:262:LYS:HB2	2.07	0.53
1:E:83:HIS:NE2	3:E:302:23J:O10	2.42	0.53
1:J:180:GLU:HG2	1:J:214:LEU:HD13	1.91	0.52
1:I:71:GLY:HA2	1:J:67:TRP:HA	1.92	0.52
1:D:83:HIS:NE2	3:D:302:23J:O10	2.43	0.52
1:J:202:ALA:HA	1:J:205:MET:SD	2.51	0.51
1:L:180:GLU:HG3	1:L:214:LEU:HD13	1.93	0.51
1:J:176:PRO:HD3	1:J:205:MET:CE	2.41	0.50
3:K:302:23J:O11	5:K:679:HOH:O	2.19	0.50
1:H:198:ASP:HB3	1:H:202:ALA:HB2	1.92	0.50
1:L:202:ALA:HA	1:L:205:MET:HG3	1.94	0.49
1:E:63:PHE:CD1	3:F:302[B]:23J:H1	2.46	0.49
1:C:70:LEU:HD21	1:C:253:PRO:HG3	1.93	0.49
1:A:63:PHE:CD1	3:B:302[A]:23J:H1	2.47	0.48
1:C:67:TRP:HA	1:D:71:GLY:HA2	1.95	0.48
1:I:13:LYS:HE2	1:J:1:MET:HG3	1.96	0.48
1:G:83:HIS:NE2	3:G:302[B]:23J:O11	2.46	0.47
1:H:83:HIS:NE2	3:H:302:23J:O10	2.47	0.47
1:I:1:MET:HA	1:I:2:SER:HA	1.58	0.47
1:B:2[B]:SER:OG	5:B:650:HOH:O	2.20	0.47
1:E:67:TRP:HA	1:F:71:GLY:HA2	1.97	0.46
1:H:202:ALA:HB1	1:H:209:PHE:HA	1.97	0.46
1:L:172:PRO:HD2	1:L:194:CYS:SG	2.55	0.46
1:L:261:PRO:O	1:L:262:LYS:HB3	2.15	0.46
1:B:190:TRP:HB3	1:B:215:LEU:HD11	1.98	0.46
1:H:172:PRO:HD2	1:H:194:CYS:SG	2.56	0.46
1:I:153:LYS:NZ	5:I:671:HOH:O	2.50	0.45
1:I:83:HIS:NE2	3:I:302:23J:O11	2.49	0.45
1:C:172:PRO:HD2	1:C:194:CYS:SG	2.56	0.45
1:J:83:HIS:NE2	3:J:302:23J:O10	2.50	0.45
1:L:133:GLU:OE1	1:L:181:TYR:OH	2.35	0.45
1:E:190:TRP:HB3	1:E:215:LEU:HD11	1.99	0.44
1:I:25:THR:HG23	1:I:76:THR:HB	1.97	0.44
1:K:71:GLY:HA2	1:L:67:TRP:HA	1.98	0.44
1:E:147:MET:HB2	1:E:190:TRP:CH2	2.52	0.44
1:C:262:LYS:HA	1:C:262:LYS:HD3	1.63	0.44
1:G:71:GLY:HA2	1:H:67:TRP:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:CE1	3:B:302[A]:23J:H1	2.53	0.44
1:C:190:TRP:HB3	1:C:215:LEU:HD11	1.99	0.44
1:J:175:THR:OG1	1:J:177:ASP:OD1	2.26	0.44
1:E:3:ALA:HB2	1:F:18:GLU:HG2	1.99	0.44
1:I:133:GLU:OE1	1:I:181:TYR:OH	2.33	0.44
5:I:533:HOH:O	1:J:1:MET:SD	2.62	0.44
1:J:261:PRO:O	1:J:262:LYS:HB2	2.17	0.44
1:H:176:PRO:HD3	1:H:205:MET:HE2	2.00	0.43
1:D:260:VAL:HG23	1:D:262:LYS:HD3	2.01	0.43
1:G:180:GLU:HG2	1:G:214:LEU:HD13	1.99	0.43
1:J:15:LEU:HA	1:J:15:LEU:HD12	1.81	0.43
1:G:1:MET:HA	1:G:2:SER:C	2.45	0.42
1:I:38:PRO:HA	1:I:39:PRO:HD3	1.90	0.42
1:J:147:MET:HB2	1:J:190:TRP:CH2	2.55	0.42
1:L:190:TRP:HB3	1:L:215:LEU:HD11	2.01	0.41
1:A:71:GLY:HA2	1:B:67:TRP:HA	2.03	0.41
1:G:38:PRO:HA	1:G:39:PRO:HD3	1.97	0.41
1:A:147:MET:HB2	1:A:190:TRP:CH2	2.55	0.41
1:D:84:TRP:CD2	1:D:212:HIS:HB3	2.56	0.41
1:K:70:LEU:HD21	1:K:253:PRO:HG2	2.03	0.41
1:C:90:TYR:CZ	1:C:219:ASN:HB2	2.56	0.41
1:H:20:GLU:OE1	1:H:262:LYS:HE3	2.21	0.41
1:I:10:LEU:HD22	1:J:10:LEU:HD22	2.02	0.41
1:F:149:THR:HG21	1:F:172:PRO:HG2	2.03	0.40
1:K:13:LYS:NZ	1:L:1:MET:O	2.47	0.40
1:E:63:PHE:CZ	3:F:302[B]:23J:H1	2.55	0.40
1:E:180:GLU:HG2	1:E:214:LEU:HD13	2.02	0.40
1:I:262:LYS:HE3	1:I:262:LYS:HB3	1.87	0.40
1:H:65:TRP:CD1	1:H:65:TRP:N	2.90	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	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	30	22
1	B	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	30	22
1	C	260/263 (99%)	252 (97%)	7 (3%)	1 (0%)	30	22
1	D	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	30	22
1	E	260/263 (99%)	256 (98%)	3 (1%)	1 (0%)	30	22
1	F	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	30	22
1	G	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	30	22
1	H	261/263 (99%)	256 (98%)	4 (2%)	1 (0%)	30	22
1	I	261/263 (99%)	255 (98%)	5 (2%)	1 (0%)	30	22
1	J	260/263 (99%)	255 (98%)	4 (2%)	1 (0%)	30	22
1	K	260/263 (99%)	254 (98%)	5 (2%)	1 (0%)	30	22
1	L	260/263 (99%)	254 (98%)	5 (2%)	1 (0%)	30	22
All	All	3125/3156 (99%)	3060 (98%)	53 (2%)	12 (0%)	30	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	60	GLY
1	J	60	GLY
1	A	60	GLY
1	B	60	GLY
1	D	60	GLY
1	E	60	GLY
1	K	60	GLY
1	C	60	GLY
1	G	60	GLY
1	H	60	GLY
1	L	60	GLY
1	F	60	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	208/207 (100%)	205 (99%)	3 (1%)	59	59
1	B	207/207 (100%)	206 (100%)	1 (0%)	81	84
1	C	207/207 (100%)	205 (99%)	2 (1%)	68	70
1	D	207/207 (100%)	206 (100%)	1 (0%)	81	84
1	E	207/207 (100%)	202 (98%)	5 (2%)	43	38
1	F	207/207 (100%)	206 (100%)	1 (0%)	81	84
1	G	207/207 (100%)	205 (99%)	2 (1%)	68	70
1	H	207/207 (100%)	205 (99%)	2 (1%)	68	70
1	I	208/207 (100%)	203 (98%)	5 (2%)	43	38
1	J	207/207 (100%)	205 (99%)	2 (1%)	68	70
1	K	207/207 (100%)	206 (100%)	1 (0%)	81	84
1	L	207/207 (100%)	206 (100%)	1 (0%)	81	84
All	All	2486/2484 (100%)	2460 (99%)	26 (1%)	68	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	TYR
1	A	65	TRP
1	A	262	LYS
1	B	65	TRP
1	C	65	TRP
1	C	262	LYS
1	D	65	TRP
1	E	1	MET
1	E	56	TYR
1	E	65	TRP
1	E	260	VAL
1	E	262	LYS
1	F	56	TYR
1	G	65	TRP
1	G	262	LYS
1	H	56	TYR
1	H	65	TRP
1	I	56	TYR
1	I	65	TRP
1	I	146	VAL
1	I	248[A]	ARG
1	I	248[B]	ARG

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Mol	Chain	Res	Type
1	J	40	ASP
1	J	65	TRP
1	K	65	TRP
1	L	65	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	212	HIS
1	H	136	HIS
1	I	4	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 43 ligands modelled in this entry, 28 are monoatomic - leaving 15 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	23J	I	302	2	12,12,12	1.01	1 (8%)	14,16,16	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	23J	H	302	2	12,12,12	2.23	2 (16%)	14,16,16	1.17	1 (7%)
3	23J	A	302	2	12,12,12	1.30	1 (8%)	14,16,16	1.15	1 (7%)
3	23J	D	302	2	12,12,12	0.92	0	14,16,16	1.14	1 (7%)
3	23J	E	302	2	12,12,12	1.51	1 (8%)	14,16,16	1.23	2 (14%)
3	23J	C	302	2	12,12,12	0.89	1 (8%)	14,16,16	1.20	2 (14%)
3	23J	F	302[A]	2	12,12,12	1.40	2 (16%)	14,16,16	1.28	3 (21%)
3	23J	F	302[B]	-	12,12,12	0.95	0	14,16,16	1.40	2 (14%)
3	23J	J	302	2	12,12,12	1.80	1 (8%)	14,16,16	1.30	3 (21%)
3	23J	L	302	2	12,12,12	1.15	2 (16%)	14,16,16	1.28	2 (14%)
3	23J	K	302	2	12,12,12	1.10	2 (16%)	14,16,16	1.11	1 (7%)
3	23J	B	302[A]	-	12,12,12	0.88	1 (8%)	14,16,16	1.05	0
3	23J	G	302[A]	-	12,12,12	0.75	1 (8%)	14,16,16	1.04	0
3	23J	B	302[B]	2	12,12,12	1.54	2 (16%)	14,16,16	1.11	1 (7%)
3	23J	G	302[B]	2	12,12,12	0.86	1 (8%)	14,16,16	1.13	2 (14%)

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	23J	I	302	2	-	0/8/8/8	0/1/1/1
3	23J	H	302	2	-	3/8/8/8	0/1/1/1
3	23J	A	302	2	-	0/8/8/8	0/1/1/1
3	23J	D	302	2	-	0/8/8/8	0/1/1/1
3	23J	E	302	2	-	0/8/8/8	0/1/1/1
3	23J	C	302	2	-	1/8/8/8	0/1/1/1
3	23J	F	302[A]	2	-	0/8/8/8	0/1/1/1
3	23J	F	302[B]	-	-	3/8/8/8	0/1/1/1
3	23J	J	302	2	-	2/8/8/8	0/1/1/1
3	23J	L	302	2	-	0/8/8/8	0/1/1/1
3	23J	K	302	2	-	3/8/8/8	0/1/1/1
3	23J	B	302[A]	-	-	0/8/8/8	0/1/1/1
3	23J	G	302[A]	-	-	1/8/8/8	0/1/1/1
3	23J	B	302[B]	2	-	3/8/8/8	0/1/1/1
3	23J	G	302[B]	2	-	0/8/8/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	302	23J	C09-C07	-7.21	1.47	1.54
3	J	302	23J	C09-C07	-5.72	1.49	1.54
3	E	302	23J	C09-C07	-4.58	1.50	1.54
3	B	302[B]	23J	C09-C07	-4.33	1.50	1.54
3	F	302[A]	23J	C09-C07	-3.80	1.51	1.54
3	A	302	23J	C09-C07	-3.60	1.51	1.54
3	L	302	23J	C09-C07	-2.87	1.52	1.54
3	K	302	23J	C09-C07	-2.78	1.52	1.54
3	B	302[B]	23J	O10-C09	-2.65	1.23	1.30
3	F	302[A]	23J	O10-C09	-2.57	1.23	1.30
3	I	302	23J	O10-C09	-2.38	1.24	1.30
3	H	302	23J	O10-C09	-2.26	1.24	1.30
3	L	302	23J	O10-C09	-2.24	1.24	1.30
3	B	302[A]	23J	O10-C09	-2.21	1.24	1.30
3	G	302[B]	23J	O10-C09	-2.21	1.24	1.30
3	C	302	23J	O10-C09	-2.18	1.24	1.30
3	K	302	23J	O10-C09	-2.08	1.24	1.30
3	G	302[A]	23J	O10-C09	-2.04	1.25	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	302	23J	O10-C09-O11	2.95	130.92	123.90
3	A	302	23J	O10-C09-O11	2.79	130.55	123.90
3	H	302	23J	O10-C09-O11	2.77	130.50	123.90
3	E	302	23J	O10-C09-O11	2.75	130.45	123.90
3	L	302	23J	O10-C09-O11	2.64	130.18	123.90
3	B	302[B]	23J	O10-C09-O11	2.41	129.64	123.90
3	L	302	23J	O11-C09-C07	-2.39	113.42	121.39
3	F	302[B]	23J	O11-C09-C07	-2.36	113.51	121.39
3	F	302[A]	23J	O10-C09-O11	2.36	129.53	123.90
3	K	302	23J	O10-C09-O11	2.35	129.49	123.90
3	F	302[A]	23J	O11-C09-C07	-2.34	113.59	121.39
3	D	302	23J	O10-C09-O11	2.33	129.45	123.90
3	F	302[B]	23J	C05-C07-C09	2.28	122.89	118.47
3	C	302	23J	O11-C09-C07	-2.18	114.13	121.39
3	C	302	23J	O10-C09-O11	2.17	129.07	123.90
3	G	302[B]	23J	O10-C09-O11	2.15	129.02	123.90
3	J	302	23J	O11-C09-C07	-2.08	114.45	121.39
3	G	302[B]	23J	O11-C09-C07	-2.05	114.56	121.39
3	J	302	23J	C06-C05-C07	-2.04	114.73	119.37
3	E	302	23J	C06-C05-C07	-2.02	114.78	119.37
3	F	302[A]	23J	C06-C05-C07	-2.01	114.80	119.37

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302[B]	23J	O08-C07-C09-O10
3	F	302[B]	23J	C05-C07-C09-O10
3	F	302[B]	23J	C05-C07-C09-O11
3	F	302[B]	23J	O08-C07-C09-O10
3	G	302[A]	23J	O08-C07-C09-O10
3	H	302	23J	O08-C07-C09-O10
3	J	302	23J	O08-C07-C09-O10
3	K	302	23J	C05-C07-C09-O10
3	K	302	23J	C05-C07-C09-O11
3	K	302	23J	O08-C07-C09-O10
3	B	302[B]	23J	C05-C07-C09-O10
3	H	302	23J	C05-C07-C09-O10
3	H	302	23J	C05-C07-C09-O11
3	B	302[B]	23J	C05-C07-C09-O11
3	C	302	23J	C05-C07-C09-O10
3	J	302	23J	C05-C07-C09-O10

There are no ring outliers.

13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	302	23J	1	0
3	H	302	23J	1	0
3	D	302	23J	1	0
3	E	302	23J	1	0
3	C	302	23J	2	0
3	F	302[A]	23J	1	0
3	F	302[B]	23J	3	0
3	J	302	23J	1	0
3	L	302	23J	1	0
3	K	302	23J	2	0
3	B	302[A]	23J	2	0
3	B	302[B]	23J	1	0
3	G	302[B]	23J	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	262/263 (99%)	-0.66	1 (0%) 88 90	10, 18, 33, 65	1 (0%)
1	B	262/263 (99%)	-0.63	1 (0%) 88 90	9, 20, 34, 57	1 (0%)
1	C	262/263 (99%)	-0.29	3 (1%) 78 80	16, 29, 45, 92	0
1	D	263/263 (100%)	-0.51	2 (0%) 82 85	13, 21, 40, 99	0
1	E	262/263 (99%)	-0.52	2 (0%) 82 85	11, 21, 37, 119	0
1	F	263/263 (100%)	-0.60	2 (0%) 82 85	11, 19, 36, 71	0
1	G	262/263 (99%)	-0.39	1 (0%) 88 90	14, 25, 41, 86	0
1	H	263/263 (100%)	-0.26	2 (0%) 82 85	15, 28, 44, 94	0
1	I	262/263 (99%)	-0.54	1 (0%) 88 90	12, 22, 36, 88	1 (0%)
1	J	262/263 (99%)	-0.53	1 (0%) 88 90	13, 22, 36, 54	0
1	K	262/263 (99%)	-0.51	1 (0%) 88 90	14, 23, 38, 104	0
1	L	262/263 (99%)	-0.55	1 (0%) 88 90	13, 21, 35, 67	0
All	All	3147/3156 (99%)	-0.50	18 (0%) 85 87	9, 22, 40, 119	3 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	263	ALA	5.1
1	D	1	MET	5.0
1	F	1	MET	4.5
1	A	1	MET	4.3
1	E	1	MET	3.9
1	K	1	MET	3.7
1	H	1	MET	3.7
1	I	1	MET	3.5
1	G	1	MET	3.4
1	B	263	ALA	2.9
1	C	1	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	L	1	MET	2.6
1	C	41	PHE	2.5
1	J	1	MET	2.2
1	D	15	LEU	2.2
1	C	262	LYS	2.1
1	E	262	LYS	2.1
1	F	263	ALA	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	23J	B	302[A]	12/12	0.74	0.22	31,33,35,112	12
3	23J	B	302[B]	12/12	0.74	0.22	24,32,33,112	12
3	23J	G	302[A]	12/12	0.80	0.26	43,45,47,156	12
3	23J	G	302[B]	12/12	0.80	0.26	37,45,45,156	12
3	23J	F	302[A]	12/12	0.84	0.13	21,29,31,42	12
3	23J	F	302[B]	12/12	0.84	0.13	16,29,31,39	12
3	23J	I	302	12/12	0.84	0.18	35,37,42,117	12
3	23J	H	302	12/12	0.85	0.16	36,39,43,158	12
3	23J	C	302	12/12	0.88	0.15	39,40,52,83	12
3	23J	E	302	12/12	0.89	0.14	32,36,40,103	12
3	23J	K	302	12/12	0.89	0.12	26,29,36,67	12
3	23J	J	302	12/12	0.91	0.15	32,35,40,140	12
3	23J	D	302	12/12	0.91	0.12	28,31,42,101	12
4	CA	C	304	1/1	0.91	0.10	81,81,81,81	0
3	23J	L	302	12/12	0.92	0.13	31,35,41,152	0
3	23J	A	302	12/12	0.92	0.12	33,34,45,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	B	305	1/1	0.93	0.11	43,43,43,43	0
4	CA	A	305	1/1	0.95	0.09	52,52,52,52	0
2	MN	H	301	1/1	0.96	0.05	24,24,24,24	0
4	CA	B	303	1/1	0.96	0.08	34,34,34,34	0
2	MN	C	301	1/1	0.96	0.05	22,22,22,22	0
4	CA	C	303	1/1	0.96	0.06	31,31,31,31	0
4	CA	A	303	1/1	0.96	0.07	36,36,36,36	0
4	CA	J	304	1/1	0.96	0.12	50,50,50,50	0
4	CA	L	305	1/1	0.96	0.11	47,47,47,47	0
4	CA	D	303	1/1	0.97	0.09	46,46,46,46	0
2	MN	B	301	1/1	0.98	0.03	17,17,17,17	0
2	MN	I	301	1/1	0.98	0.04	16,16,16,16	0
2	MN	K	301	1/1	0.98	0.04	20,20,20,20	0
2	MN	L	301	1/1	0.98	0.03	17,17,17,17	0
2	MN	D	301	1/1	0.98	0.04	18,18,18,18	0
4	CA	I	303	1/1	0.98	0.03	21,21,21,21	0
2	MN	E	301	1/1	0.98	0.03	15,15,15,15	0
4	CA	L	304	1/1	0.98	0.07	35,35,35,35	0
2	MN	G	301	1/1	0.98	0.03	22,22,22,22	0
2	MN	A	301	1/1	0.99	0.02	14,14,14,14	0
4	CA	F	303	1/1	0.99	0.01	21,21,21,21	0
4	CA	B	304	1/1	0.99	0.02	23,23,23,23	0
4	CA	J	303	1/1	0.99	0.03	26,26,26,26	0
2	MN	J	301	1/1	0.99	0.03	18,18,18,18	0
4	CA	L	303	1/1	0.99	0.03	23,23,23,23	0
4	CA	A	304	1/1	0.99	0.07	22,22,22,22	0
2	MN	F	301	1/1	0.99	0.03	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.