



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:39 AM GMT

PDB ID : 3BJK  
Title : Crystal structure of HI0827, a hexameric broad specificity acyl-coenzyme A thioesterase: The Asp44Ala mutant enzyme  
Authors : Willis, M.A.; Herzberg, O.; Structure 2 Function Project (S2F)  
Deposited on : 2007-12-04  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

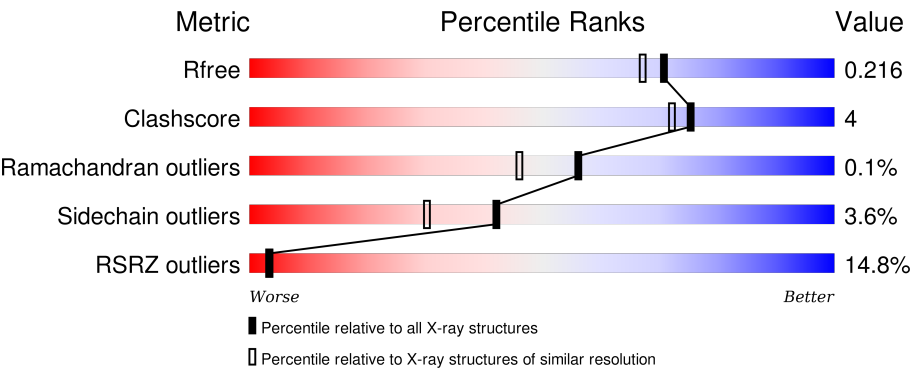
# 1 Overall quality at a glance i

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 <sub>free</sub>	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	153	<div><div>9%</div><div><div></div><div></div><div></div><div></div></div><div>78%12%• 8%</div></div>
1	B	153	<div><div>20%</div><div><div></div><div></div><div></div><div></div></div><div>88%5%• 7%</div></div>
1	C	153	<div><div>17%</div><div><div></div><div></div><div></div><div></div></div><div>82%11%7%</div></div>
1	D	153	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>77%12%• 9%</div></div>
1	E	153	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>82%8%• 8%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	153	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	A	1	-	-	-	X
2	CIT	A	155	-	-	-	X
2	CIT	D	155	-	-	-	X
3	EDO	A	156	-	-	-	X
3	EDO	B	158	-	-	-	X
3	EDO	D	161	-	-	-	X
3	EDO	D	162	-	-	-	X
3	EDO	E	157	-	-	-	X
3	EDO	E	158	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6970 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.

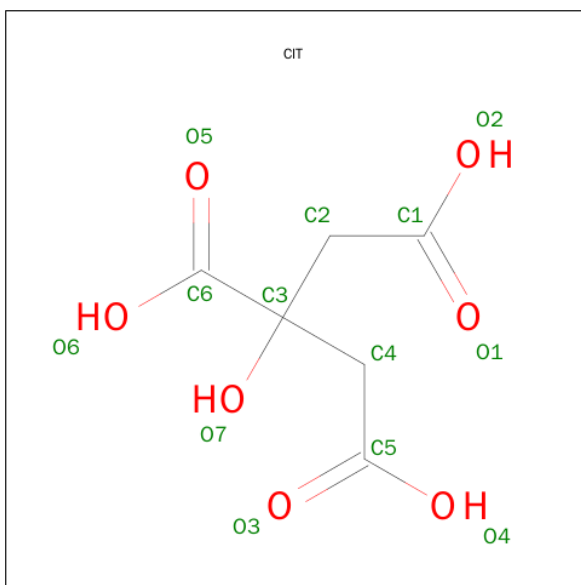
- Molecule 1 is a protein called Acyl-CoA thioester hydrolase HI0827.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1058	667	185	197	9			
1	B	142	Total	C	N	O	S	0	0	0
			1072	675	189	199	9			
1	C	143	Total	C	N	O	S	0	0	1
			1080	679	191	201	9			
1	D	139	Total	C	N	O	S	0	1	0
			1054	665	184	196	9			
1	E	140	Total	C	N	O	S	0	0	0
			1058	667	185	197	9			
1	F	139	Total	C	N	O	S	0	0	1
			1046	661	183	193	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	ASP	ENGINEERED	UNP P44886
B	44	ALA	ASP	ENGINEERED	UNP P44886
C	44	ALA	ASP	ENGINEERED	UNP P44886
D	44	ALA	ASP	ENGINEERED	UNP P44886
E	44	ALA	ASP	ENGINEERED	UNP P44886
F	44	ALA	ASP	ENGINEERED	UNP P44886

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	C	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	D	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0
3	E	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		

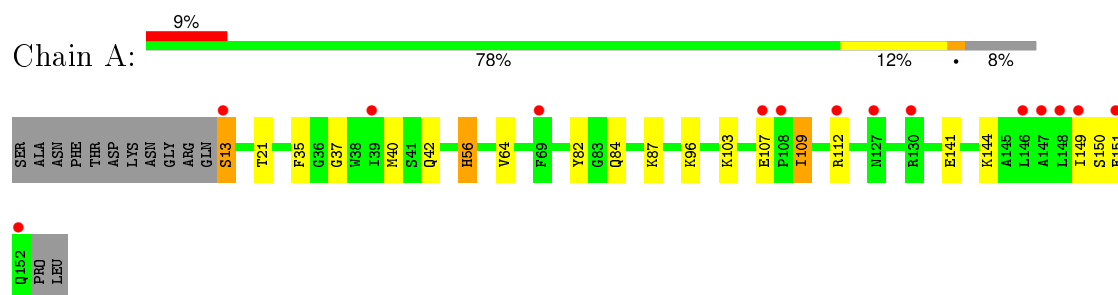
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total	O	0	0
			89	89		
4	B	77	Total	O	0	0
			77	77		
4	C	77	Total	O	0	0
			77	77		
4	D	98	Total	O	0	0
			98	98		
4	E	77	Total	O	0	0
			77	77		
4	F	45	Total	O	0	0
			45	45		

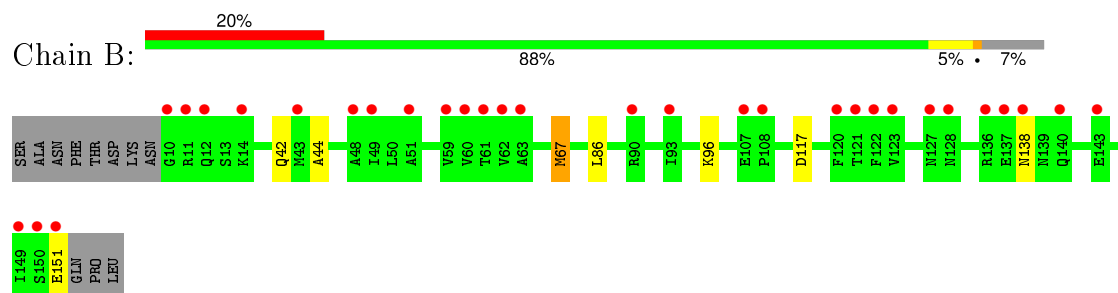
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

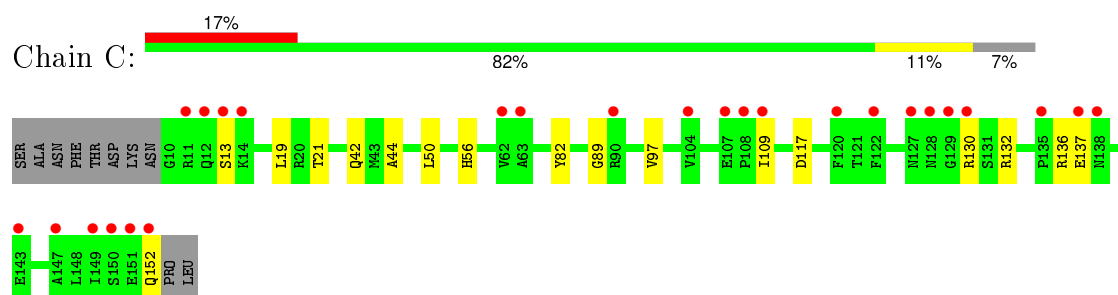
- Molecule 1: Acyl-CoA thioester hydrolase HI0827



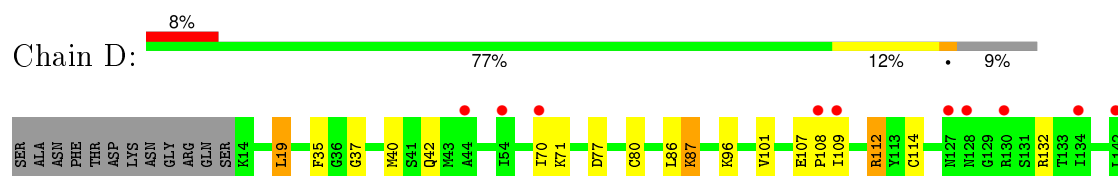
- Molecule 1: Acyl-CoA thioester hydrolase HI0827



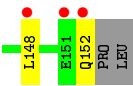
- Molecule 1: Acyl-CoA thioester hydrolase HI0827



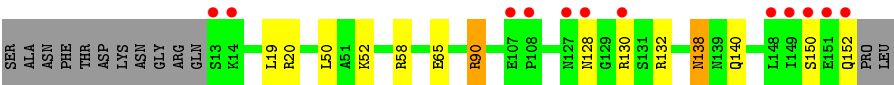
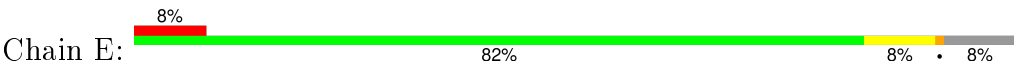
- Molecule 1: Acyl-CoA thioester hydrolase HI0827



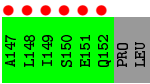
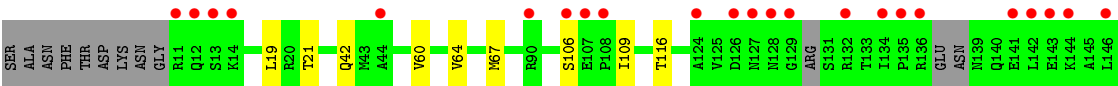
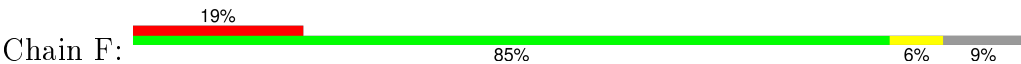




● Molecule 1: Acyl-CoA thioester hydrolase HI0827



● Molecule 1: Acyl-CoA thioester hydrolase HI0827



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.49 Å   63.11 Å   104.72 Å 90.00°   100.14°   90.00°	Depositor
Resolution (Å)	29.88 – 1.90 29.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.88-1.90) 98.0 (29.87-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 1.91 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.169   ,   0.210 0.177   ,   0.216	Depositor DCC
$R_{free}$ test set	6357 reflections (8.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 78120 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6970	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: EDO, CIT

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	0.90	0/1072	0.84	0/1447
1	B	0.88	0/1086	0.86	1/1465 (0.1%)
1	C	0.93	1/1094 (0.1%)	0.87	2/1475 (0.1%)
1	D	0.98	1/1072 (0.1%)	0.90	3/1447 (0.2%)
1	E	0.89	1/1072 (0.1%)	0.92	5/1447 (0.3%)
1	F	0.74	0/1058	0.77	0/1424
All	All	0.89	3/6454 (0.0%)	0.86	11/8705 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	152	GLN	C-O	11.04	1.44	1.23
1	C	137	GLU	CD-OE1	6.83	1.33	1.25
1	D	80	CYS	CB-SG	-6.41	1.71	1.82

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	67	MET	CA-CB-CG	7.32	125.74	113.30
1	D	77	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	E	90	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	E	90	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	E	132	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	117	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	19	LEU	CA-CB-CG	5.84	128.74	115.30
1	E	58	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	E	20	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	132	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	1058	0	1090	18	0
1	B	1072	0	1104	5	0
1	C	1080	0	1112	6	0
1	D	1054	0	1086	16	0
1	E	1058	0	1090	7	0
1	F	1046	0	1080	4	0
2	A	26	0	10	2	0
2	D	13	0	5	0	0
3	A	24	0	36	1	0
3	B	16	0	24	1	0
3	C	12	0	18	0	0
3	D	28	0	42	7	0
3	E	16	0	24	2	0
3	F	4	0	6	0	0
4	A	89	0	0	7	0
4	B	77	0	0	1	0
4	C	77	0	0	1	0
4	D	98	0	0	4	0
4	E	77	0	0	3	1
4	F	45	0	0	1	0
All	All	6970	0	6727	52	1

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 4.

All (52) 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:D:114:CYS:O	3:D:160:EDO:H11	1.86	0.74
1:A:144:LYS:NZ	4:A:187:HOH:O	2.26	0.69
1:A:87:LYS:HD3	4:A:202:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:GLN:OE1	4:D:296:HOH:O	2.13	0.66
1:E:19:LEU:CD2	4:E:212:HOH:O	2.43	0.66
1:D:42:GLN:HG2	4:D:296:HOH:O	1.97	0.64
1:A:107:GLU:O	4:A:229:HOH:O	2.16	0.61
1:C:42:GLN:HG2	4:C:166:HOH:O	2.03	0.58
1:E:19:LEU:HD22	4:E:212:HOH:O	2.03	0.58
1:A:21:THR:HA	1:D:19:LEU:HD22	1.86	0.57
1:D:107:GLU:OE1	1:D:108:PRO:HA	2.04	0.56
1:D:96:LYS:HD3	3:D:161:EDO:H21	1.87	0.56
1:A:84:GLN:NE2	1:A:96:LYS:HD3	2.20	0.56
1:D:96:LYS:HG2	3:D:161:EDO:H12	1.89	0.55
2:A:155:CIT:O7	2:A:155:CIT:O2	2.17	0.55
1:D:96:LYS:HD3	3:D:161:EDO:C2	2.37	0.54
1:A:84:GLN:HE22	1:A:96:LYS:HD3	1.73	0.53
1:D:114:CYS:O	3:D:160:EDO:C1	2.56	0.52
1:D:35:PHE:CE2	1:D:37:GLY:HA3	2.46	0.51
1:E:19:LEU:HD23	4:E:212:HOH:O	2.11	0.50
1:B:42:GLN:HG2	4:B:174:HOH:O	2.12	0.49
1:D:86:LEU:C	1:D:87:LYS:HG2	2.32	0.48
1:A:56:HIS:HE1	1:A:141:GLU:OE1	1.96	0.48
1:F:64:VAL:HG11	1:F:67:MET:CE	2.44	0.48
1:A:56:HIS:HD2	3:A:160:EDO:O2	1.96	0.48
1:A:103:LYS:HE3	4:A:229:HOH:O	2.14	0.47
2:A:155:CIT:H41	4:A:220:HOH:O	2.14	0.47
1:A:42:GLN:HG2	4:A:179:HOH:O	2.15	0.47
1:E:138:ASN:HD22	1:E:138:ASN:N	2.12	0.47
1:D:114:CYS:HB3	3:D:160:EDO:H11	1.97	0.46
1:E:50:LEU:HD21	3:E:156:EDO:H21	1.97	0.46
1:B:86:LEU:HD23	3:B:158:EDO:H22	1.96	0.46
1:C:19:LEU:HD22	1:F:21:THR:HA	1.97	0.45
1:C:44:ALA:HB2	1:D:40:MET:HE1	1.98	0.45
1:A:35:PHE:CE2	1:A:37:GLY:HA3	2.52	0.44
1:E:52:LYS:HZ3	3:E:158:EDO:C2	2.31	0.44
1:C:89:GLY:O	1:C:136:ARG:NH2	2.51	0.43
1:A:40:MET:HE1	1:B:44:ALA:HB2	2.01	0.43
1:A:84:GLN:HG3	4:A:204:HOH:O	2.19	0.43
1:A:64:VAL:HB	1:B:67:MET:HB3	2.00	0.43
1:D:101:VAL:O	1:D:112:ARG:HA	2.19	0.42
1:B:96:LYS:NZ	1:B:117:ASP:HB2	2.34	0.42
3:D:157:EDO:H12	4:D:281:HOH:O	2.19	0.42
1:F:42:GLN:HG2	4:F:167:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:ASN:HD22	1:E:130:ARG:NH2	2.18	0.41
1:A:149:ILE:O	1:A:151:GLU:N	2.53	0.41
1:A:13:SER:HB3	1:A:82:TYR:CE2	2.55	0.41
1:A:56:HIS:O	1:D:109:ILE:HD13	2.21	0.41
1:D:70:ILE:HG22	1:D:71:LYS:HG3	2.01	0.41
1:A:109:ILE:CD1	4:D:238:HOH:O	2.68	0.41
1:C:21:THR:HA	1:F:19:LEU:HD22	2.03	0.40
1:C:82:TYR:O	1:C:97:VAL:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:207:HOH:O	4:E:234:HOH:O[2_545]	1.81	0.39

## 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	138/153 (90%)	136 (99%)	1 (1%)	1 (1%)	26	14
1	B	140/153 (92%)	139 (99%)	1 (1%)	0	100	100
1	C	141/153 (92%)	139 (99%)	2 (1%)	0	100	100
1	D	138/153 (90%)	138 (100%)	0	0	100	100
1	E	138/153 (90%)	138 (100%)	0	0	100	100
1	F	133/153 (87%)	131 (98%)	2 (2%)	0	100	100
All	All	828/918 (90%)	821 (99%)	6 (1%)	1 (0%)	56	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	SER

### 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	116/127 (91%)	112 (97%)	4 (3%)	44	33
1	B	117/127 (92%)	115 (98%)	2 (2%)	68	64
1	C	118/127 (93%)	112 (95%)	6 (5%)	29	17
1	D	116/127 (91%)	112 (97%)	4 (3%)	44	33
1	E	116/127 (91%)	111 (96%)	5 (4%)	35	23
1	F	114/127 (90%)	110 (96%)	4 (4%)	43	31
All	All	697/762 (92%)	672 (96%)	25 (4%)	42	30

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	56	HIS
1	A	109	ILE
1	A	112	ARG
1	B	138	ASN
1	B	151	GLU
1	C	13	SER
1	C	50	LEU
1	C	56	HIS
1	C	109	ILE
1	C	130	ARG
1	C	152	GLN
1	D	87	LYS
1	D	112	ARG
1	D	148	LEU
1	D	152	GLN
1	E	65	GLU
1	E	90	ARG

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Mol	Chain	Res	Type
1	E	138	ASN
1	E	140	GLN
1	E	150	SER
1	F	60	VAL
1	F	106	SER
1	F	109	ILE
1	F	116	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	B	138	ASN
1	C	12	GLN
1	C	42	GLN
1	C	152	GLN
1	D	42	GLN
1	D	152	GLN
1	E	84	GLN
1	E	128	ASN
1	E	138	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

28 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	CIT	A	1	-	3,12,12	2.01	1 (33%)	3,17,17	1.06	0
2	CIT	A	155	-	3,12,12	1.59	1 (33%)	3,17,17	5.60	2 (66%)
3	EDO	A	156	-	3,3,3	0.67	0	2,2,2	0.43	0
3	EDO	A	157	-	3,3,3	0.74	0	2,2,2	0.28	0
3	EDO	A	158	-	3,3,3	0.55	0	2,2,2	0.69	0
3	EDO	A	159	-	3,3,3	0.97	0	2,2,2	0.56	0
3	EDO	A	160	-	3,3,3	0.53	0	2,2,2	0.55	0
3	EDO	A	161	-	3,3,3	0.59	0	2,2,2	0.30	0
3	EDO	B	155	-	3,3,3	0.51	0	2,2,2	0.08	0
3	EDO	B	156	-	3,3,3	0.71	0	2,2,2	0.22	0
3	EDO	B	157	-	3,3,3	0.48	0	2,2,2	0.56	0
3	EDO	B	158	-	3,3,3	0.61	0	2,2,2	0.24	0
3	EDO	C	155	-	3,3,3	0.59	0	2,2,2	0.23	0
3	EDO	C	156	-	3,3,3	0.65	0	2,2,2	0.37	0
3	EDO	C	157	-	3,3,3	0.55	0	2,2,2	0.17	0
2	CIT	D	155	-	3,12,12	1.67	1 (33%)	3,17,17	1.49	0
3	EDO	D	156	-	3,3,3	0.51	0	2,2,2	0.16	0
3	EDO	D	157	-	3,3,3	0.42	0	2,2,2	0.46	0
3	EDO	D	158	-	3,3,3	0.93	0	2,2,2	0.46	0
3	EDO	D	159	-	3,3,3	0.54	0	2,2,2	0.26	0
3	EDO	D	160	-	3,3,3	0.87	0	2,2,2	0.93	0
3	EDO	D	161	-	3,3,3	0.62	0	2,2,2	0.73	0
3	EDO	D	162	-	3,3,3	0.58	0	2,2,2	0.22	0
3	EDO	E	155	-	3,3,3	0.50	0	2,2,2	0.54	0
3	EDO	E	156	-	3,3,3	0.35	0	2,2,2	0.51	0
3	EDO	E	157	-	3,3,3	0.57	0	2,2,2	0.18	0
3	EDO	E	158	-	3,3,3	0.66	0	2,2,2	0.41	0
3	EDO	F	155	-	3,3,3	0.69	0	2,2,2	0.12	0

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	CIT	A	1	-	-	0/6/16/16	0/0/0/0
2	CIT	A	155	-	-	0/6/16/16	0/0/0/0
3	EDO	A	156	-	-	0/1/1/1	0/0/0/0
3	EDO	A	157	-	-	0/1/1/1	0/0/0/0
3	EDO	A	158	-	-	0/1/1/1	0/0/0/0
3	EDO	A	159	-	-	0/1/1/1	0/0/0/0
3	EDO	A	160	-	-	0/1/1/1	0/0/0/0
3	EDO	A	161	-	-	0/1/1/1	0/0/0/0
3	EDO	B	155	-	-	0/1/1/1	0/0/0/0
3	EDO	B	156	-	-	0/1/1/1	0/0/0/0
3	EDO	B	157	-	-	0/1/1/1	0/0/0/0
3	EDO	B	158	-	-	0/1/1/1	0/0/0/0
3	EDO	C	155	-	-	0/1/1/1	0/0/0/0
3	EDO	C	156	-	-	0/1/1/1	0/0/0/0
3	EDO	C	157	-	-	0/1/1/1	0/0/0/0
2	CIT	D	155	-	-	0/6/16/16	0/0/0/0
3	EDO	D	156	-	-	0/1/1/1	0/0/0/0
3	EDO	D	157	-	-	0/1/1/1	0/0/0/0
3	EDO	D	158	-	-	0/1/1/1	0/0/0/0
3	EDO	D	159	-	-	0/1/1/1	0/0/0/0
3	EDO	D	160	-	-	0/1/1/1	0/0/0/0
3	EDO	D	161	-	-	0/1/1/1	0/0/0/0
3	EDO	D	162	-	-	0/1/1/1	0/0/0/0
3	EDO	E	155	-	-	0/1/1/1	0/0/0/0
3	EDO	E	156	-	-	0/1/1/1	0/0/0/0
3	EDO	E	157	-	-	0/1/1/1	0/0/0/0
3	EDO	E	158	-	-	0/1/1/1	0/0/0/0
3	EDO	F	155	-	-	0/1/1/1	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	155	CIT	O7-C3	2.53	1.47	1.43
2	D	155	CIT	O7-C3	2.54	1.47	1.43
2	A	1	CIT	O7-C3	3.27	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	155	CIT	C3-C2-C1	-9.14	100.34	114.96
2	A	155	CIT	C3-C4-C5	-3.14	109.93	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	155	CIT	2	0
3	A	160	EDO	1	0
3	B	158	EDO	1	0
3	D	157	EDO	1	0
3	D	160	EDO	3	0
3	D	161	EDO	3	0
3	E	156	EDO	1	0
3	E	158	EDO	1	0

## 5.7 Other polymers

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	140/153 (91%)	0.75	14 (10%) 9 10	26, 32, 48, 59	0
1	B	142/153 (92%)	1.22	31 (21%) 1 1	26, 32, 46, 51	0
1	C	143/153 (93%)	0.99	26 (18%) 2 2	27, 32, 48, 57	0
1	D	139/153 (90%)	0.97	13 (9%) 11 12	26, 32, 45, 54	0
1	E	140/153 (91%)	0.84	12 (8%) 13 14	27, 32, 45, 58	0
1	F	139/153 (90%)	1.28	29 (20%) 1 1	27, 33, 44, 57	0
All	All	843/918 (91%)	1.01	125 (14%) 3 3	26, 32, 46, 59	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	LEU	8.8
1	E	13	SER	8.5
1	F	12	GLN	8.1
1	F	136	ARG	7.9
1	B	138	ASN	7.6
1	F	128	ASN	6.5
1	B	150	SER	6.3
1	A	13	SER	6.1
1	B	137	GLU	5.9
1	F	152	GLN	5.9
1	E	150	SER	5.6
1	C	12	GLN	5.6
1	B	12	GLN	5.4
1	C	127	ASN	5.4
1	E	151	GLU	5.3
1	F	90	ARG	5.0
1	B	108	PRO	5.0
1	F	149	ILE	4.9
1	E	130	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	152	GLN	4.7
1	F	11	ARG	4.4
1	A	151	GLU	4.3
1	C	151	GLU	4.2
1	E	149	ILE	4.3
1	B	90	ARG	4.2
1	C	137	GLU	4.2
1	F	142	LEU	4.0
1	F	146	LEU	4.0
1	F	148	LEU	3.9
1	F	14	LYS	3.9
1	C	13	SER	3.8
1	E	107	GLU	3.8
1	D	152	GLN	3.8
1	C	108	PRO	3.7
1	A	149	ILE	3.5
1	D	109	ILE	3.5
1	C	135	PRO	3.5
1	C	152	GLN	3.5
1	F	143	GLU	3.5
1	D	148	LEU	3.5
1	D	151	GLU	3.4
1	D	128	ASN	3.4
1	E	14	LYS	3.3
1	B	121	THR	3.3
1	C	150	SER	3.3
1	B	136	ARG	3.3
1	F	135	PRO	3.2
1	D	70	ILE	3.2
1	F	129	GLY	3.2
1	F	126	ASP	3.2
1	B	140	GLN	3.2
1	F	127	ASN	3.2
1	B	127	ASN	3.1
1	B	151	GLU	3.1
1	B	120	PHE	3.1
1	F	107	GLU	3.1
1	E	108	PRO	3.0
1	B	143	GLU	3.0
1	C	149	ILE	3.0
1	A	127	ASN	2.9
1	A	146	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	123	VAL	2.9
1	A	152	GLN	2.9
1	B	128	ASN	2.9
1	B	149	ILE	2.9
1	C	138	ASN	2.9
1	B	107	GLU	2.9
1	F	134	ILE	2.9
1	B	122	PHE	2.8
1	F	106	SER	2.8
1	E	128	ASN	2.8
1	F	151	GLU	2.8
1	C	63	ALA	2.8
1	E	148	LEU	2.8
1	B	14	LYS	2.8
1	B	62	VAL	2.7
1	D	108	PRO	2.7
1	C	107	GLU	2.7
1	F	144	LYS	2.6
1	D	44	ALA	2.6
1	C	11	ARG	2.6
1	F	147	ALA	2.6
1	F	132	ARG	2.6
1	F	13	SER	2.6
1	C	128	ASN	2.6
1	E	127	ASN	2.5
1	F	141	GLU	2.5
1	D	127	ASN	2.5
1	C	62	VAL	2.5
1	B	61	THR	2.5
1	B	10	GLY	2.5
1	B	51	ALA	2.5
1	F	150	SER	2.5
1	F	108	PRO	2.5
1	B	59	VAL	2.5
1	C	104	VAL	2.4
1	C	14	LYS	2.4
1	D	142	LEU	2.4
1	C	109	ILE	2.4
1	C	143	GLU	2.4
1	B	93	ILE	2.3
1	A	112	ARG	2.3
1	B	11	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	129	GLY	2.2
1	B	60	VAL	2.2
1	B	43	MET	2.2
1	A	147	ALA	2.2
1	C	90	ARG	2.2
1	A	107	GLU	2.2
1	B	48	ALA	2.1
1	B	49	ILE	2.1
1	C	147	ALA	2.1
1	A	69	PHE	2.1
1	C	122	PHE	2.1
1	A	39	ILE	2.1
1	D	54	ILE	2.1
1	A	130	ARG	2.0
1	C	120	PHE	2.0
1	B	63	ALA	2.0
1	F	44	ALA	2.0
1	C	130	ARG	2.0
1	D	130	ARG	2.0
1	F	124	ALA	2.0
1	A	108	PRO	2.0
1	D	134	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CIT	A	155	13/13	0.85	0.33	7.10	30,41,45,46	0
3	EDO	D	161	4/4	0.90	0.38	6.28	36,40,40,43	0
2	CIT	D	155	13/13	0.89	0.33	5.00	28,42,50,54	0
3	EDO	E	157	4/4	0.88	0.17	4.55	51,52,52,53	0
3	EDO	D	162	4/4	0.88	0.18	3.10	47,49,49,50	0
3	EDO	B	158	4/4	0.86	0.43	3.07	49,51,51,52	0
2	CIT	A	1	13/13	0.90	0.24	2.78	29,33,36,37	0
3	EDO	E	158	4/4	0.86	0.19	2.67	44,47,47,47	0
3	EDO	A	156	4/4	0.92	0.17	2.13	23,27,30,31	0
3	EDO	A	161	4/4	0.92	0.21	1.87	35,40,40,41	0
3	EDO	B	157	4/4	0.86	0.22	1.85	46,49,49,50	0
3	EDO	E	156	4/4	0.95	0.24	1.60	34,38,40,40	0
3	EDO	A	158	4/4	0.82	0.24	1.57	36,40,42,45	0
3	EDO	C	156	4/4	0.92	0.19	1.22	33,41,42,43	0
3	EDO	D	160	4/4	0.93	0.20	1.04	33,37,37,40	0
3	EDO	D	156	4/4	0.92	0.15	0.58	25,30,31,35	0
3	EDO	C	155	4/4	0.93	0.17	0.41	35,36,37,37	0
3	EDO	A	157	4/4	0.89	0.16	0.24	35,38,38,40	0
3	EDO	B	155	4/4	0.92	0.15	0.00	26,27,29,30	0
3	EDO	F	155	4/4	0.81	0.15	-0.01	45,47,47,48	0
3	EDO	A	159	4/4	0.89	0.17	-0.26	32,37,37,39	0
3	EDO	E	155	4/4	0.94	0.13	-0.76	35,37,38,41	0
3	EDO	B	156	4/4	0.90	0.11	-1.09	42,44,45,45	0
3	EDO	D	159	4/4	0.96	0.10	-1.36	24,26,26,26	0
3	EDO	D	158	4/4	0.93	0.13	-1.37	29,31,31,33	0
3	EDO	C	157	4/4	0.92	0.28	-	48,50,50,51	0
3	EDO	D	157	4/4	0.92	0.22	-	26,34,37,39	0
3	EDO	A	160	4/4	0.90	0.28	-	35,37,40,41	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.