



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 01:12 PM GMT

PDB ID : 3MLP
Title : Early B-cell Factor 1 (Ebf1) bound to DNA
Authors : Treiber, N.; Treiber, T.; Zocher, G.; Grosschedl, R.
Deposited on : 2010-04-17
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

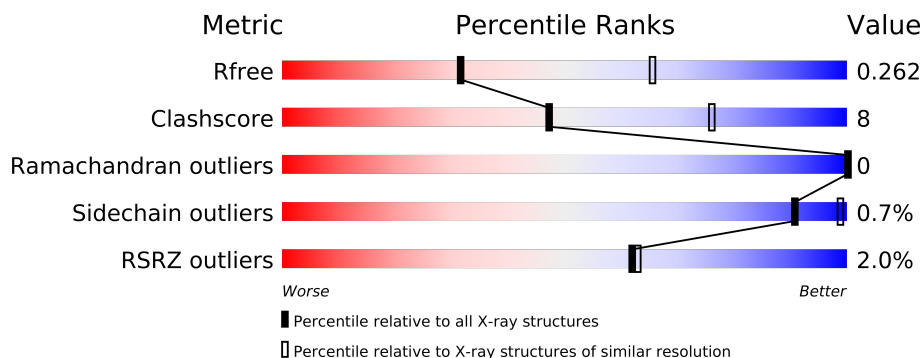
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	402	
1	B	402	
1	E	402	
1	F	402	
2	C	22	
2	D	22	
2	G	22	
2	H	22	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11961 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transcription factor COE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2626	1653	475	482	16			
1	B	332	Total	C	N	O	S	0	0	0
			2591	1637	462	477	15			
1	E	303	Total	C	N	O	S	0	0	0
			2399	1511	435	438	15			
1	F	298	Total	C	N	O	S	0	0	0
			2334	1475	415	429	15			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	DELETION	UNP Q07802
A	?	-	THR	DELETION	UNP Q07802
A	?	-	PRO	DELETION	UNP Q07802
A	?	-	SER	DELETION	UNP Q07802
A	?	-	TYR	DELETION	UNP Q07802
A	?	-	LEU	DELETION	UNP Q07802
A	?	-	GLU	DELETION	UNP Q07802
A	252	ALA	HIS	ENGINEERED MUTATION	UNP Q07802
A	415	ALA	-	EXPRESSION TAG	UNP Q07802
A	416	ALA	-	EXPRESSION TAG	UNP Q07802
A	417	VAL	-	EXPRESSION TAG	UNP Q07802
A	418	LEU	-	EXPRESSION TAG	UNP Q07802
A	419	GLU	-	EXPRESSION TAG	UNP Q07802
A	420	HIS	-	EXPRESSION TAG	UNP Q07802
A	421	HIS	-	EXPRESSION TAG	UNP Q07802
A	422	HIS	-	EXPRESSION TAG	UNP Q07802
A	423	HIS	-	EXPRESSION TAG	UNP Q07802
A	424	HIS	-	EXPRESSION TAG	UNP Q07802
A	425	HIS	-	EXPRESSION TAG	UNP Q07802
B	?	-	GLY	DELETION	UNP Q07802
B	?	-	THR	DELETION	UNP Q07802

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	DELETION	UNP Q07802
B	?	-	SER	DELETION	UNP Q07802
B	?	-	TYR	DELETION	UNP Q07802
B	?	-	LEU	DELETION	UNP Q07802
B	?	-	GLU	DELETION	UNP Q07802
B	252	ALA	HIS	ENGINEERED MUTATION	UNP Q07802
B	415	ALA	-	EXPRESSION TAG	UNP Q07802
B	416	ALA	-	EXPRESSION TAG	UNP Q07802
B	417	VAL	-	EXPRESSION TAG	UNP Q07802
B	418	LEU	-	EXPRESSION TAG	UNP Q07802
B	419	GLU	-	EXPRESSION TAG	UNP Q07802
B	420	HIS	-	EXPRESSION TAG	UNP Q07802
B	421	HIS	-	EXPRESSION TAG	UNP Q07802
B	422	HIS	-	EXPRESSION TAG	UNP Q07802
B	423	HIS	-	EXPRESSION TAG	UNP Q07802
B	424	HIS	-	EXPRESSION TAG	UNP Q07802
B	425	HIS	-	EXPRESSION TAG	UNP Q07802
E	?	-	GLY	DELETION	UNP Q07802
E	?	-	THR	DELETION	UNP Q07802
E	?	-	PRO	DELETION	UNP Q07802
E	?	-	SER	DELETION	UNP Q07802
E	?	-	TYR	DELETION	UNP Q07802
E	?	-	LEU	DELETION	UNP Q07802
E	?	-	GLU	DELETION	UNP Q07802
E	252	ALA	HIS	ENGINEERED MUTATION	UNP Q07802
E	415	ALA	-	EXPRESSION TAG	UNP Q07802
E	416	ALA	-	EXPRESSION TAG	UNP Q07802
E	417	VAL	-	EXPRESSION TAG	UNP Q07802
E	418	LEU	-	EXPRESSION TAG	UNP Q07802
E	419	GLU	-	EXPRESSION TAG	UNP Q07802
E	420	HIS	-	EXPRESSION TAG	UNP Q07802
E	421	HIS	-	EXPRESSION TAG	UNP Q07802
E	422	HIS	-	EXPRESSION TAG	UNP Q07802
E	423	HIS	-	EXPRESSION TAG	UNP Q07802
E	424	HIS	-	EXPRESSION TAG	UNP Q07802
E	425	HIS	-	EXPRESSION TAG	UNP Q07802
F	?	-	GLY	DELETION	UNP Q07802
F	?	-	THR	DELETION	UNP Q07802
F	?	-	PRO	DELETION	UNP Q07802
F	?	-	SER	DELETION	UNP Q07802
F	?	-	TYR	DELETION	UNP Q07802
F	?	-	LEU	DELETION	UNP Q07802

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLU	DELETION	UNP Q07802
F	252	ALA	HIS	ENGINEERED MUTATION	UNP Q07802
F	415	ALA	-	EXPRESSION TAG	UNP Q07802
F	416	ALA	-	EXPRESSION TAG	UNP Q07802
F	417	VAL	-	EXPRESSION TAG	UNP Q07802
F	418	LEU	-	EXPRESSION TAG	UNP Q07802
F	419	GLU	-	EXPRESSION TAG	UNP Q07802
F	420	HIS	-	EXPRESSION TAG	UNP Q07802
F	421	HIS	-	EXPRESSION TAG	UNP Q07802
F	422	HIS	-	EXPRESSION TAG	UNP Q07802
F	423	HIS	-	EXPRESSION TAG	UNP Q07802
F	424	HIS	-	EXPRESSION TAG	UNP Q07802
F	425	HIS	-	EXPRESSION TAG	UNP Q07802

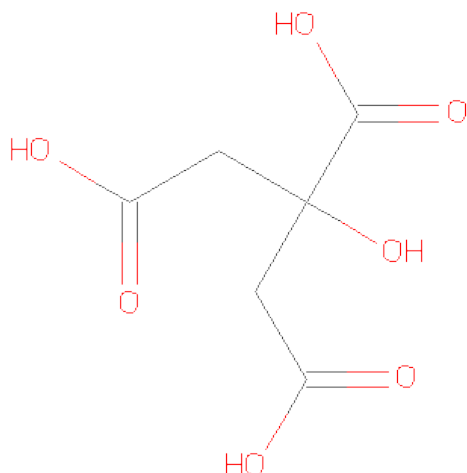
- Molecule 2 is a DNA chain called DNA (5'-D(*CP*TP*TP*TP*AP*TP*TP*CP*CP*CP*AP*TP*GP*GP*GP*AP*AP*TP*AP*AP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			448	216	81	130	21			
2	D	22	Total	C	N	O	P	0	0	0
			448	216	81	130	21			
2	G	22	Total	C	N	O	P	0	0	0
			448	216	81	130	21			
2	H	22	Total	C	N	O	P	0	0	0
			448	216	81	130	21			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	E	1	Total	C	O	0	0
			13	6	7		
4	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	36	Total	O	0	0
			36	36		
5	B	24	Total	O	0	0
			24	24		
5	C	3	Total	O	0	0
			3	3		
5	D	4	Total	O	0	0
			4	4		
5	E	34	Total	O	0	0
			34	34		
5	F	35	Total	O	0	0
			35	35		
5	G	8	Total	O	0	0
			8	8		

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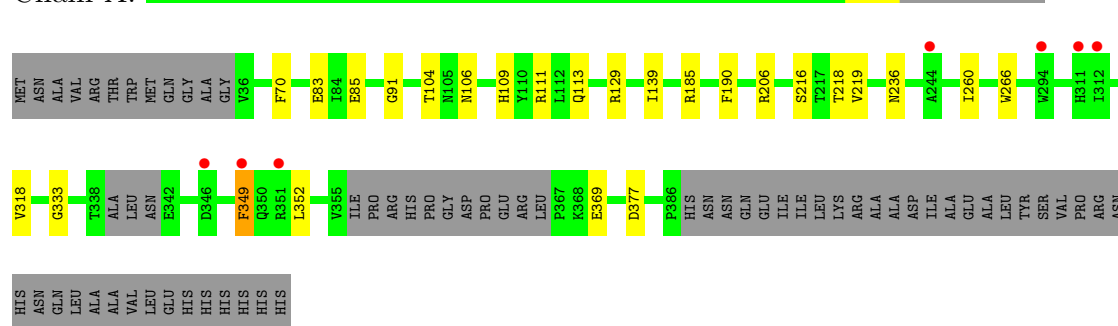
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	6	Total	O	0	0
			6	6		

3 Residue-property plots

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.

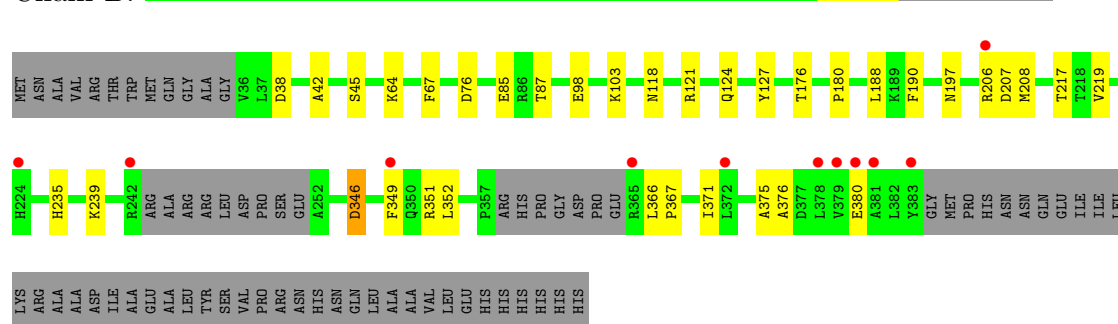
• Molecule 1: Transcription factor COE1

Chain A:



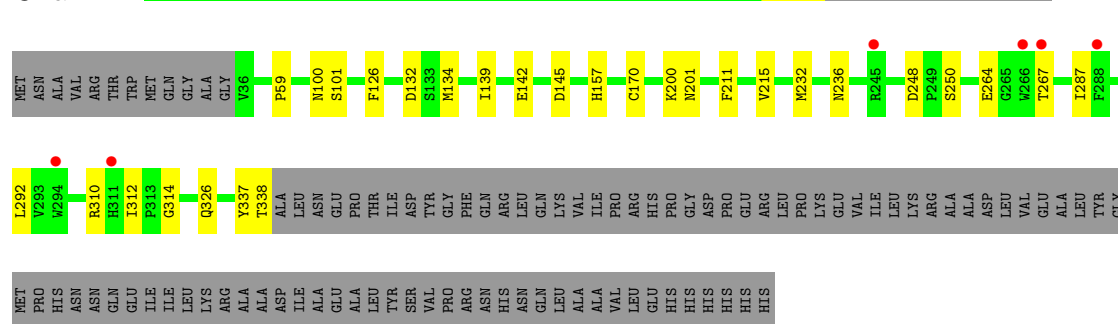
• Molecule 1: Transcription factor COE1

Chain B:



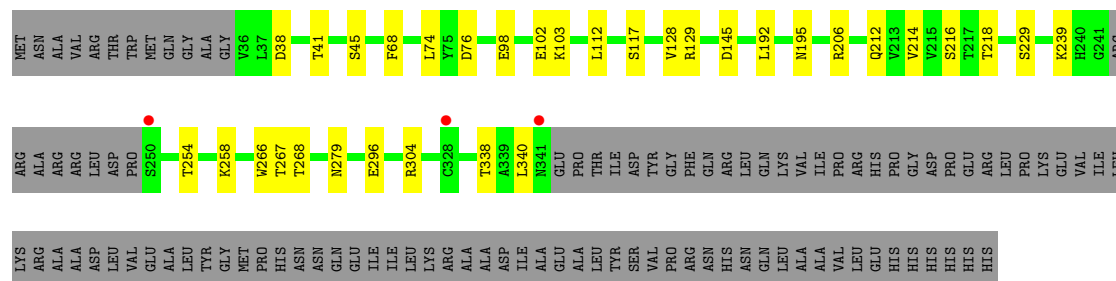
• Molecule 1: Transcription factor COE1

Chain E:



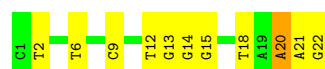
• Molecule 1: Transcription factor COE1

Chain F: 



- Molecule 2: DNA (5'-D(*CP*TP*TP*TP*AP*TP*TP*CP*CP*CP*AP*TP*GP*GP*GP*AP*AP*TP*AP*AP*AP*G)-3')

Chain C: 



- Molecule 2: DNA (5'-D(*CP*TP*TP*TP*AP*TP*TP*CP*CP*CP*AP*TP*GP*GP*GP*AP*AP*TP*AP*AP*AP*G)-3')

Chain D: 



- Molecule 2: DNA (5'-D(*CP*TP*TP*TP*AP*TP*TP*CP*CP*CP*AP*TP*GP*GP*GP*AP*AP*TP*AP*AP*AP*G)-3')

Chain G: 



- Molecule 2: DNA (5'-D(*CP*TP*TP*TP*AP*TP*TP*CP*CP*CP*AP*TP*GP*GP*GP*AP*AP*TP*AP*AP*AP*G)-3')

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.49Å 78.69Å 103.57Å 88.99° 90.00° 77.81°	Depositor
Resolution (Å)	38.75 – 2.80 38.75 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.75-2.80) 96.8 (38.75-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.204 , 0.264 0.204 , 0.262	Depositor DCC
R_{free} test set	2592 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 20.1	EDS
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 51836 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11961	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.49	0/2681	0.64	0/3626
1	B	0.48	0/2646	0.65	0/3583
1	E	0.53	0/2451	0.66	0/3314
1	F	0.52	0/2384	0.67	0/3226
2	C	0.97	0/502	1.77	13/773 (1.7%)
2	D	1.17	1/502 (0.2%)	1.84	16/773 (2.1%)
2	G	0.97	0/502	1.71	9/773 (1.2%)
2	H	1.01	1/502 (0.2%)	1.69	13/773 (1.7%)
All	All	0.62	2/12170 (0.0%)	0.96	51/16841 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6	DT	C3'-O3'	-6.87	1.35	1.44
2	H	12	DT	C3'-O3'	-6.05	1.36	1.44

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	18	DT	O4'-C4'-C3'	-9.72	100.17	106.00
2	D	6	DT	N3-C4-O4	9.02	125.31	119.90
2	H	7	DT	N3-C4-O4	8.95	125.27	119.90
2	G	6	DT	O4'-C4'-C3'	-8.89	100.66	106.00
2	D	6	DT	C5-C4-O4	-8.87	118.69	124.90

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2626	0	0	20	0
1	B	2591	0	0	26	0
1	E	2399	0	0	17	0
1	F	2334	0	0	20	0
2	C	448	0	0	4	0
2	D	448	0	0	3	0
2	G	448	0	0	1	0
2	H	448	0	0	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	26	0	10	4	0
4	B	13	0	5	2	0
4	E	13	0	5	0	0
4	F	13	0	5	0	0
5	A	36	0	0	1	0
5	B	24	0	0	0	0
5	C	3	0	0	1	0
5	D	4	0	0	0	0
5	E	34	0	0	1	0
5	F	35	0	0	3	0
5	G	8	0	0	0	0
5	H	6	0	0	0	0
All	All	11961	0	25	90	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 90 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:LYS:NZ	1:B:197:ASN:OD1	1.87	1.08
1:F:239:LYS:NZ	2:H:15:DG:N7	2.27	0.82
1:A:206:ARG:NH1	2:C:21:DA:OP1	2.16	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:349:PHE:O	1:A:352:LEU:CB	2.32	0.77
1:B:85:GLU:OE1	1:B:121:ARG:NH1	2.19	0.75

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	331/402 (82%)	306 (92%)	25 (8%)	0	100	100
1	B	326/402 (81%)	305 (94%)	21 (6%)	0	100	100
1	E	301/402 (75%)	284 (94%)	17 (6%)	0	100	100
1	F	294/402 (73%)	278 (95%)	16 (5%)	0	100	100
All	All	1252/1608 (78%)	1173 (94%)	79 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	282/348 (81%)	280 (99%)	2 (1%)	91	99
1	B	279/348 (80%)	278 (100%)	1 (0%)	95	99
1	E	265/348 (76%)	262 (99%)	3 (1%)	84	98
1	F	256/348 (74%)	254 (99%)	2 (1%)	89	98
All	All	1082/1392 (78%)	1074 (99%)	8 (1%)	91	99

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	145	ASP
1	F	340	LEU
1	E	326	GLN
1	B	346	ASP
1	E	264	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\# Z > 2$
4	CIT	A	1	-	12,12,12	1.13	0	17,17,17	2.01	2 (11%)
4	CIT	A	3	-	12,12,12	0.92	0	17,17,17	1.83	5 (29%)
4	CIT	B	4	-	12,12,12	1.14	0	17,17,17	1.98	4 (23%)
4	CIT	E	2	-	12,12,12	1.08	0	17,17,17	1.85	3 (17%)
4	CIT	F	6	-	12,12,12	1.34	2 (16%)	17,17,17	2.34	7 (41%)

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
4	CIT	A	1	-	-	0/16/16/16	0/0/0/0
4	CIT	A	3	-	-	1/16/16/16	0/0/0/0
4	CIT	B	4	-	-	1/16/16/16	0/0/0/0
4	CIT	E	2	-	-	0/16/16/16	0/0/0/0
4	CIT	F	6	-	-	0/16/16/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	6	CIT	C4-C3	2.23	1.56	1.53
4	F	6	CIT	C2-C3	2.05	1.56	1.53

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4	CIT	O6-C6-C3	6.11	121.77	112.89
4	A	1	CIT	O6-C6-C3	5.86	121.41	112.89
4	F	6	CIT	O6-C6-C3	5.31	120.62	112.89
4	E	2	CIT	O6-C6-C3	5.17	120.41	112.89
4	A	3	CIT	O6-C6-C3	5.04	120.22	112.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	4	CIT	O7-C3-C6-O6
4	A	3	CIT	O7-C3-C6-O6

There are no ring outliers.

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, 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	337/402 (83%)	-0.32	7 (2%) 60 61	22, 49, 117, 155	0
1	B	332/402 (82%)	-0.27	11 (3%) 44 45	29, 48, 111, 158	0
1	E	303/402 (75%)	-0.38	6 (1%) 62 63	23, 44, 94, 140	0
1	F	298/402 (74%)	-0.47	3 (1%) 79 79	22, 44, 83, 127	0
2	C	22/22 (100%)	-0.87	0 100 100	26, 34, 59, 71	0
2	D	22/22 (100%)	-0.84	0 100 100	24, 38, 60, 88	0
2	G	22/22 (100%)	-0.90	0 100 100	24, 30, 58, 67	0
2	H	22/22 (100%)	-0.86	0 100 100	22, 33, 53, 76	0
All	All	1358/1696 (80%)	-0.39	27 (1%) 62 63	22, 46, 106, 158	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	311	HIS	3.8
1	B	378	LEU	3.8
1	E	266	TRP	3.7
1	B	379	VAL	3.6
1	B	381	ALA	3.5

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CIT	F	6	13/13	0.19	0.41	52,59,62,63	0
4	CIT	A	1	13/13	0.13	-0.24	42,46,50,51	0
4	CIT	A	3	13/13	0.12	-0.43	56,63,66,68	0
4	CIT	B	4	13/13	0.19	-0.51	61,68,71,71	0
3	ZN	E	501	1/1	0.10	-1.02	38,38,38,38	0
4	CIT	E	2	13/13	0.10	-1.28	53,56,60,60	0
3	ZN	B	501	1/1	0.10	-1.36	38,38,38,38	0
3	ZN	F	501	1/1	0.09	-1.82	32,32,32,32	0
3	ZN	A	501	1/1	0.07	-1.83	43,43,43,43	0

6.5 Other polymers

There are no such residues in this entry.