wwPDB X-ray Structure Validation Summary Report (i)

Aug 8, 2023 – 06:38 PM EDT

PDB ID	:	1PO3
Title	:	Crystal structure of ferric citrate transporter FecA in complex with ferric citrate
Authors	:	Yue, W.W.; Grizot, S.; Buchanan, S.K.
Deposited on	:	2003-06-13
Resolution	:	3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

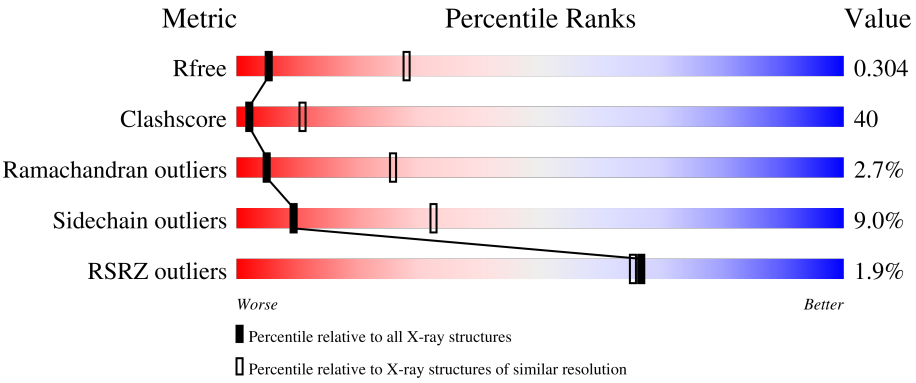
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

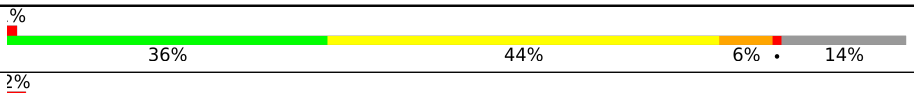
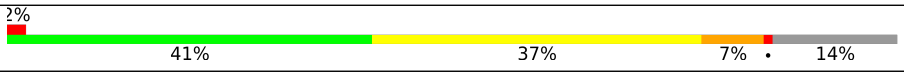
The reported resolution of this entry is 3.40 Å.

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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	751	
1	B	751	

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	FLC	A	742	-	X	X	-
2	FLC	A	743	-	X	-	-
2	FLC	B	743	-	X	-	-

2 Entry composition (i)

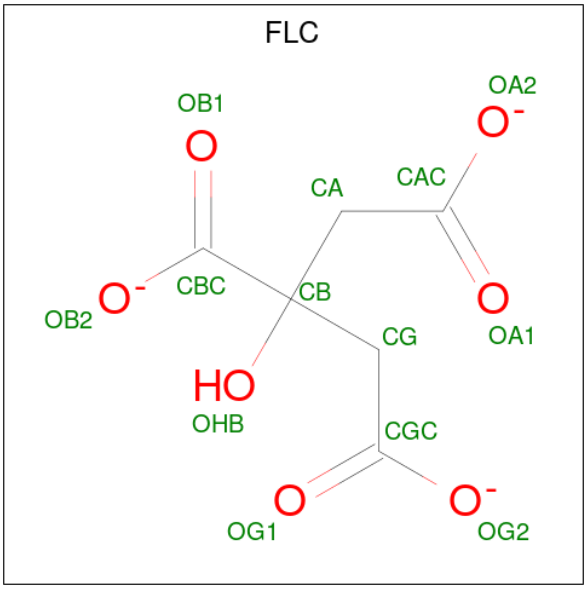
There are 3 unique types of molecules in this entry. The entry contains 10024 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Iron(III) dicitrate transport protein fecA precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	647	Total	C	N	O	S	0	0	0
			4998	3127	880	979	12			
1	B	645	Total	C	N	O	S	0	0	0
			4970	3107	879	974	10			

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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	B	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

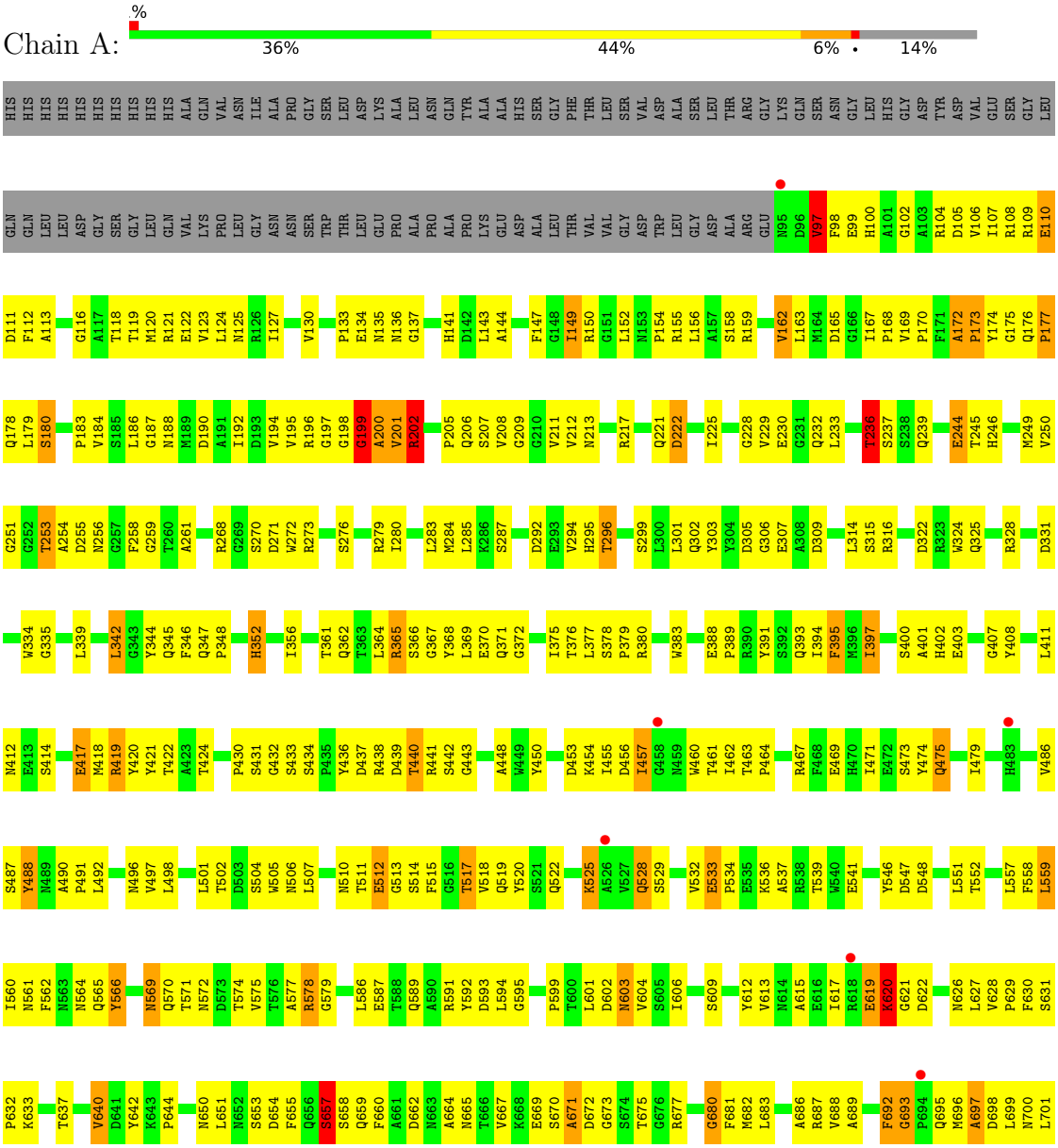
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Fe 2 2	0	0
3	B	2	Total Fe 2 2	0	0

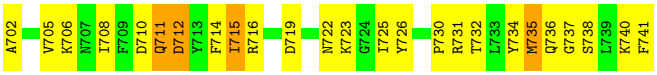
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Iron(III) dicitrate transport protein fecA precursor

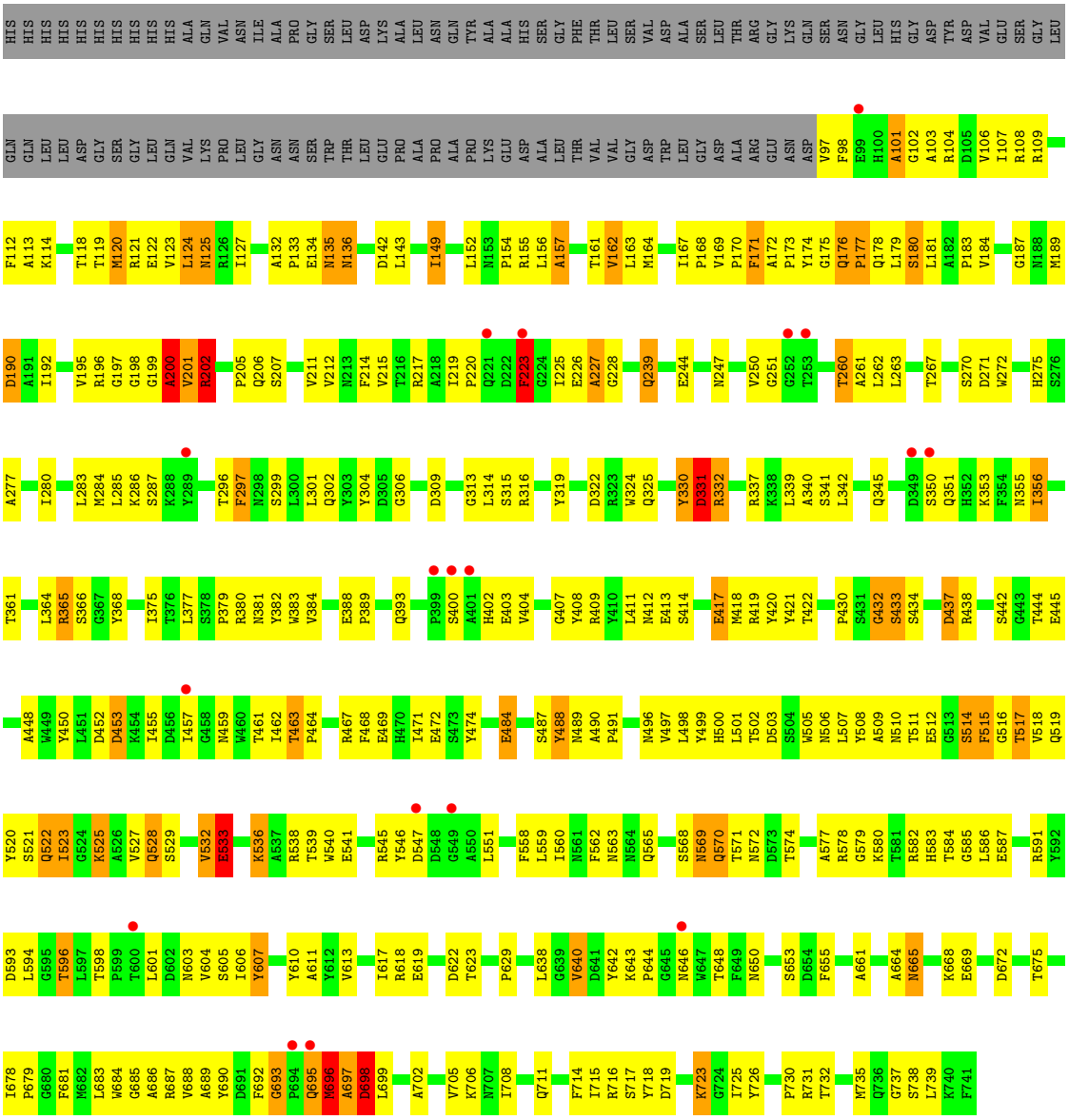
Chain A:





• Molecule 1: Iron(III) dicitrate transport protein fecA precursor

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.49Å 147.00Å 96.13Å 90.00° 110.58° 90.00°	Depositor
Resolution (Å)	15.00 – 3.40 19.77 – 3.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.40) 99.2 (19.77-3.28)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 3.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.314 0.240 , 0.304	Depositor DCC
R_{free} test set	1532 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å^2)	70.2	Xtriage
Anisotropy	0.451	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10024	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FLC, FE

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	0.75	5/5125 (0.1%)	0.86	14/6966 (0.2%)
1	B	0.66	5/5095 (0.1%)	0.89	19/6925 (0.3%)
All	All	0.70	10/10220 (0.1%)	0.88	33/13891 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	173	PRO	N-CD	-29.89	1.06	1.47
1	A	173	PRO	N-CA	17.61	1.77	1.47
1	B	697	ALA	N-CA	17.17	1.80	1.46
1	B	696	MET	C-N	16.48	1.72	1.34
1	A	200	ALA	N-CA	13.82	1.74	1.46

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	697	ALA	N-CA-CB	-18.41	84.33	110.10
1	A	200	ALA	N-CA-CB	-16.93	86.40	110.10
1	A	173	PRO	N-CA-CB	-10.01	91.29	103.30
1	B	331	ASP	O-C-N	-9.55	107.42	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	331	ASP	C-N-CA	-9.44	98.11	121.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	GLY	Peptide
1	B	200	ALA	Peptide
1	B	223	PHE	Sidechain

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	4998	0	4673	408	0
1	B	4970	0	4651	371	0
2	A	26	0	9	5	0
2	B	26	0	8	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	10024	0	9341	779	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 40.

The worst 5 of 779 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:A:200:ALA:N	1:A:200:ALA:CA	1.74	1.46
1:B:696:MET:C	1:B:697:ALA:N	1.72	1.44
1:B:697:ALA:N	1:B:697:ALA:CA	1.80	1.43
1:A:173:PRO:N	1:A:173:PRO:CA	1.77	1.35
1:A:692:PHE:HE1	1:A:701:LEU:HD12	1.17	1.08

There are no symmetry-related clashes.

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	645/751 (86%)	552 (86%)	73 (11%)	20 (3%)	4 23
1	B	643/751 (86%)	556 (86%)	72 (11%)	15 (2%)	6 28
All	All	1288/1502 (86%)	1108 (86%)	145 (11%)	35 (3%)	5 26

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	97	VAL
1	A	110	GLU
1	A	619	GLU
1	A	620	LYS
1	B	200	ALA

5.3.2 Protein sidechains (i)

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	517/617 (84%)	476 (92%)	41 (8%)	12 39
1	B	513/617 (83%)	461 (90%)	52 (10%)	7 27
All	All	1030/1234 (84%)	937 (91%)	93 (9%)	9 32

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	239	GLN

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Mol	Chain	Res	Type
1	B	502	THR
1	B	260	THR
1	B	365	ARG
1	B	517	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	496	ASN
1	B	695	GLN
1	B	500	HIS
1	B	589	GLN
1	A	569	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 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	$\#\|Z\|>2$
2	FLC	A	742	3	12,12,12	3.62	3 (25%)	17,17,17	6.89	9 (52%)
2	FLC	A	743	3	12,12,12	4.69	6 (50%)	17,17,17	6.45	8 (47%)
2	FLC	B	742	3	12,12,12	5.57	6 (50%)	17,17,17	6.76	8 (47%)
2	FLC	B	743	3	12,12,12	3.89	6 (50%)	17,17,17	6.30	10 (58%)

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	FLC	A	742	3	-	10/16/16/16	-
2	FLC	A	743	3	-	10/16/16/16	-
2	FLC	B	742	3	-	3/16/16/16	-
2	FLC	B	743	3	-	5/16/16/16	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	742	FLC	CA-CB	11.28	1.67	1.53
2	B	742	FLC	CB-CBC	10.98	1.64	1.53
2	A	743	FLC	CG-CB	10.17	1.66	1.53
2	B	743	FLC	CA-CB	9.99	1.66	1.53
2	B	742	FLC	CG-CB	9.72	1.65	1.53

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	742	FLC	OHB-CB-CBC	-22.38	77.45	108.86
2	B	742	FLC	OHB-CB-CBC	-19.96	80.83	108.86
2	A	743	FLC	OHB-CB-CBC	-19.76	81.13	108.86
2	B	743	FLC	OHB-CB-CBC	-17.67	84.06	108.86
2	B	743	FLC	OHB-CB-CG	-13.11	78.71	109.40

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	742	FLC	CAC-CA-CB-CBC
2	A	742	FLC	CG-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
2	A	742	FLC	CG-CB-CBC-OB2
2	A	742	FLC	OHB-CB-CBC-OB1
2	A	742	FLC	OHB-CB-CBC-OB2

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	742	FLC	5	0
2	B	742	FLC	2	0
2	B	743	FLC	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	696:MET	C	697:ALA	N	1.72
1	B	533:GLU	C	534:PRO	N	1.13

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^{th} 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	647/751 (86%)	-0.35	6 (0%)	84	83	9, 49, 87, 117	0
1	B	645/751 (85%)	-0.15	18 (2%)	53	51	15, 60, 99, 128	0
All	All	1292/1502 (86%)	-0.25	24 (1%)	66	65	9, 54, 96, 128	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	694	PRO	6.3
1	A	694	PRO	4.5
1	B	252	GLY	4.5
1	A	95	ASN	3.9
1	B	600	THR	3.6

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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	FE	B	745	1/1	0.84	0.10	73,73,73,73	0
2	FLC	A	743	13/13	0.94	0.20	56,56,56,56	0
2	FLC	A	742	13/13	0.94	0.21	56,56,56,56	0
2	FLC	B	742	13/13	0.95	0.22	56,56,56,56	0
3	FE	A	745	1/1	0.97	0.03	44,44,44,44	0
2	FLC	B	743	13/13	0.97	0.17	56,56,56,56	0
3	FE	B	744	1/1	0.99	0.09	37,37,37,37	0
3	FE	A	744	1/1	0.99	0.14	40,40,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.