



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:34 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

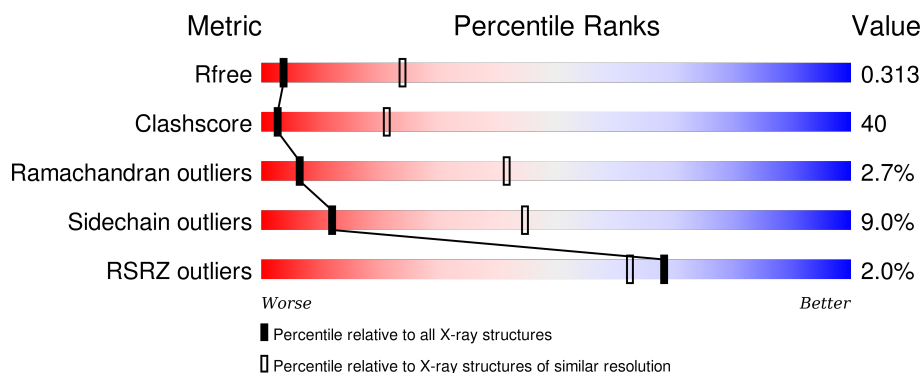
1 Overall quality at a glance ⓘ

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}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	751	<div> <div></div> <div>36% 44% 6% • 14%</div> </div>
1	B	751	<div> <div>3%</div> <div>41% 37% 7% • 14%</div> </div>

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	-

2 Entry composition [i](#)

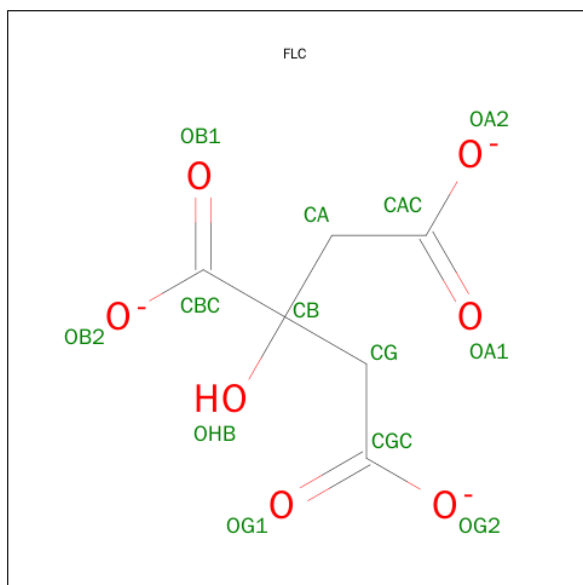
There are 3 unique types of molecules in this entry. The entry contains 10024 atoms, of which 0 are hydrogens and 0 are deuteriums.

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		

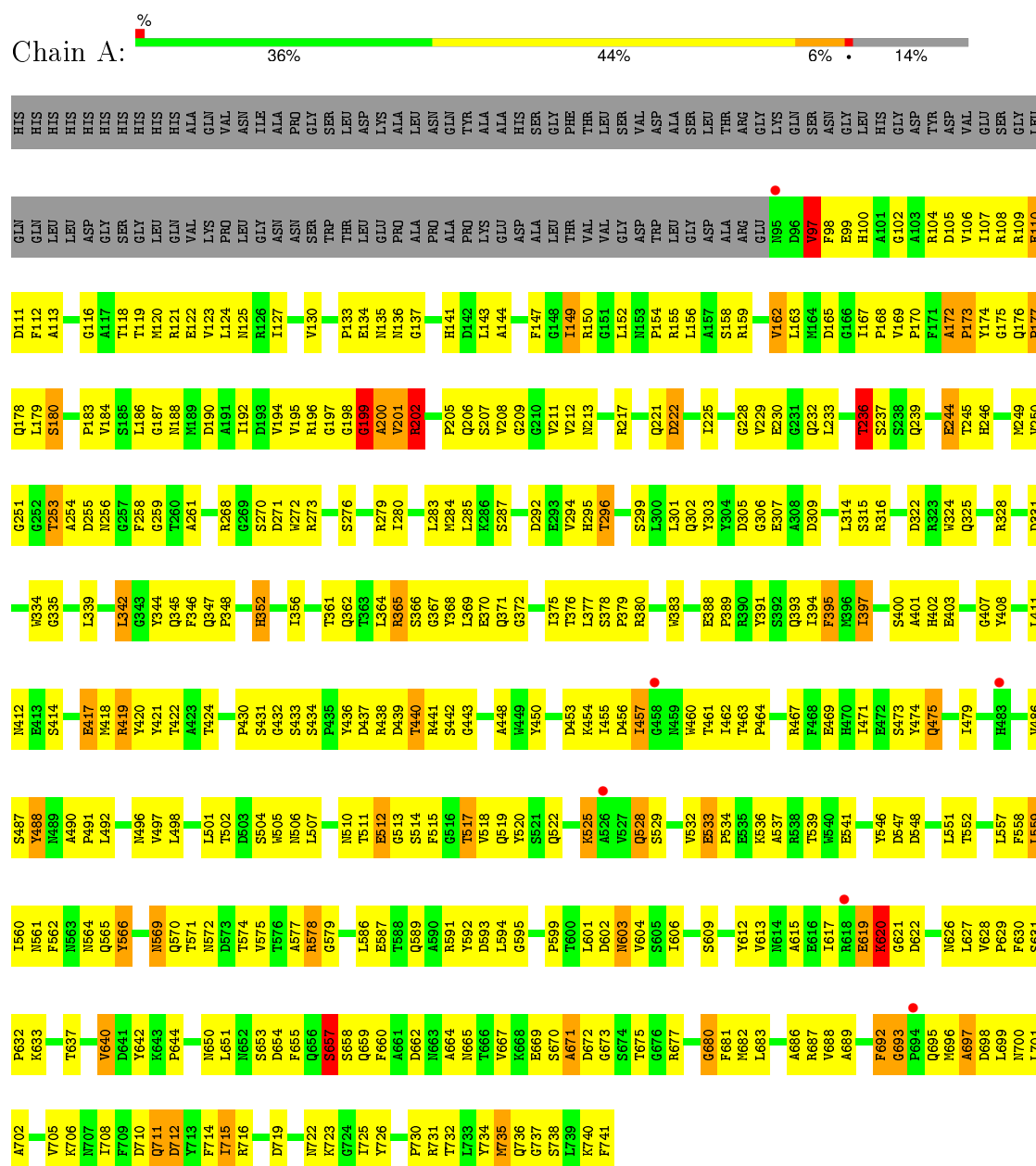
- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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: Iron(III) dicitrate transport protein fecA precursor



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

HIS	F112	D190	S276	T361	E445	Q619	Y592	I678	GLN
HIS	A191	I192	A277	L364	A448	Y520	D593	P679	GLN
HIS	K114		L280	R365	Y449	S521	L594	P679	LEU
HIS	T118	Y195	L283	R366	Y450	Q522	G595	G680	LEU
HIS	T119	A196	L284	G367	L451	Y523	T596	F681	ASP
HIS	R120	G197	L285	G368	D452	K526	T598	L683	GLY
HIS	M211	G198	K286	Y368	D453	A526	P599	P684	GLY
HIS	E122	G199	S287	K454	K455	V527	T600	G685	LEU
HIS	V123	A200	K288	I375	I455	Q528	L601	A686	GLN
ALA	L124	V201	K288	T376	D456	S529	T602	P687	VAL
GLN	M125	K262	Y289	L377	I457		H603	P688	LYS
VAL	R126			S378	G458	V532	H604	P689	PRO
ASN	I127	P205	T296	P379	M459	Q533	P604	A689	VAL
ILE		Q206	T297	R380	M460	E533	S605	P690	LEU
ALA	A132	S207	H298	N381	T461	K536	T606	D691	GLY
ASN	P133		S299	Y382	I462	A537	Y607	F692	ASN
PRO	E134	Y211	L300	N383	T463	R538		G693	GLY
GLY	E136	V212	Q302	V384	P464	T539	Y610	P694	TRP
SER	M135	L301	L302			W540	A611	Q695	SER
LEU	N136	T213	H401	E388	P467	E541	V613	P696	LEU
ASP	T143	F214	Y303	Q389	R468			L697	ASP
LEU	D142	Y215	D305	Q393	E469	R545	T617	L699	LEU
LYS	L143	T216	G306		H470	Y546	R618	A702	ALA
ALA		R217		P399	I471	D547	B619		LEU
PRO	T149	A218	D309	S399	E472	D548	T622	Y705	PRO
ASN	L152	P220	G313	A401	S473	G549	T623	W706	ASN
GLN	N153	Q221	L314	H402	Y474	A550	Y629	I708	GLN
ALA	P154	D222	S315	E403		L551			ALA
GLU	R155	G224	R316	V404	E484				GLU
HIS	A157	I225	Y319	G407	S487	P558	L638	Q711	HIS
SER		E226		Y408	Y488	L559	L639	F714	SER
THR	T161	A227	D322	R409	M489	N561	V640	T715	THR
LEU	V162	G228	R323	Y410	A490	S562	P641	R716	LEU
SER	L163		K325	L411	P491	N563	K642	S717	SER
VAL	M164	Q239	W324	M412		E564	P644	T719	VAL
ASP		E244	Q325	E413	M496	P565	G645		ASP
ASP	I167		Y330	E413	Y497	S568	N646	K723	ASP
LEU	P169		D331	S414	L498	N569	T647	F724	LEU
GLY	P170		R332	E417	H500	Q570	T648	T725	GLY
ALA	F171			M418	L501	T571	N650	Y726	ALA
ARG	A172	V250	R337	R419	T502	N572			ARG
GLY	T172	G251	K338	Y420	D503	D573			GLY
ASN	P173	G252	Y421	Y421	S504	T574	S653	P730	ASN
GLN	Y174	T253	A340	T422	H505		P654	R731	GLN
SER	G175	A254	S341		N506		P655	T732	SER
ASN	Q176		L342	P430	L507	A577			ASN
GLY	P177	T260	L342	S431	L507	H578	A611	M735	GLY
LEU	Q178	A261	Q345	G432	Y508	S579	T650	Q736	LEU
HIS	A101	L262		S433	A509	K580	T581	T737	HIS
GLY	S180	L263		S434	N510	T582	P665	S738	GLY
ASP	L181	L263	P349	S434	T511	H583		L739	ASP
A103			S350	D437	E512	T584	K668	R740	A103
T104	A182	T267							

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.49 Å 147.00 Å 96.13 Å 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
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.29 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.314 0.247 , 0.313	Depositor DCC
R_{free} test set	1532 reflections (5.33%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 33661 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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(°)	Ideal(°)
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(°)	Ideal(°)
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

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:CA	1:A:200:ALA:N	1.74	1.46
1:B:696:MET:C	1:B:697:ALA:N	1.72	1.44
1:B:697:ALA:CA	1:B:697:ALA:N	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

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	645/751 (86%)	552 (86%)	73 (11%)	20 (3%)	5	39
1	B	643/751 (86%)	556 (86%)	72 (11%)	15 (2%)	8	45
All	All	1288/1502 (86%)	1108 (86%)	145 (11%)	35 (3%)	6	41

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

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%)	15	52
1	B	513/617 (83%)	461 (90%)	52 (10%)	9	38
All	All	1030/1234 (84%)	937 (91%)	93 (9%)	12	45

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

Mol	Chain	Res	Type
1	B	108	ARG

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Mol	Chain	Res	Type
1	B	176	GLN
1	B	665	ASN
1	B	120	MET
1	B	136	ASN

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

Mol	Chain	Res	Type
1	A	700	ASN
1	B	240	ASN
1	B	656	GLN
1	A	711	GLN
1	B	136	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](#)

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	3,12,12	4.47	2 (66%)	3,17,17	3.57	2 (66%)
2	FLC	A	743	3	3,12,12	6.20	2 (66%)	3,17,17	3.82	3 (100%)
2	FLC	B	742	3	3,12,12	6.59	2 (66%)	3,17,17	5.56	2 (66%)
2	FLC	B	743	3	3,12,12	5.06	2 (66%)	3,17,17	3.36	2 (66%)

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	-	0/6/16/16	0/0/0/0
2	FLC	A	743	3	-	0/6/16/16	0/0/0/0
2	FLC	B	742	3	-	0/6/16/16	0/0/0/0
2	FLC	B	743	3	-	0/6/16/16	0/0/0/0

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	743	FLC	CG-CB	4.32	1.61	1.54
2	A	742	FLC	CA-CB	5.46	1.63	1.54
2	A	742	FLC	CG-CB	5.49	1.63	1.54
2	A	743	FLC	CA-CB	7.34	1.65	1.54
2	B	742	FLC	CG-CB	7.38	1.65	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	743	FLC	CG-CB-CA	2.70	116.25	109.81
2	B	743	FLC	CG-CB-CA	3.94	119.22	109.81
2	A	743	FLC	CB-CG-CGC	3.98	121.33	114.96
2	B	743	FLC	CB-CA-CAC	4.14	121.58	114.96
2	A	742	FLC	CB-CA-CAC	4.36	121.93	114.96

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	647/751 (86%)	-0.34	6 (0%) 85 81	9, 49, 87, 117	0
1	B	645/751 (85%)	-0.13	20 (3%) 52 48	15, 60, 99, 128	0
All	All	1292/1502 (86%)	-0.23	26 (2%) 68 62	9, 54, 96, 128	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	694	PRO	6.6
1	A	694	PRO	4.6
1	B	252	GLY	4.4
1	A	95	ASN	3.9
1	B	600	THR	3.8

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	FLC	B	742	13/13	0.95	0.22	0.59	56,56,56,56	0
2	FLC	A	742	13/13	0.94	0.21	0.46	56,56,56,56	0
2	FLC	A	743	13/13	0.94	0.20	0.17	56,56,56,56	0
2	FLC	B	743	13/13	0.97	0.17	-0.36	56,56,56,56	0
3	FE	B	745	1/1	0.84	0.10	-	73,73,73,73	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
3	FE	A	745	1/1	0.97	0.03	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.