



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:57 PM GMT

PDB ID : 6CSC
Title : CHICKEN CITRATE SYNTHASE COMPLEX WITH TRIFLUOROACET
ONYL-COA AND CITRATE
Authors : Usher, K.C.; Remington, S.J.
Deposited on : 1997-06-19
Resolution : 2.25 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

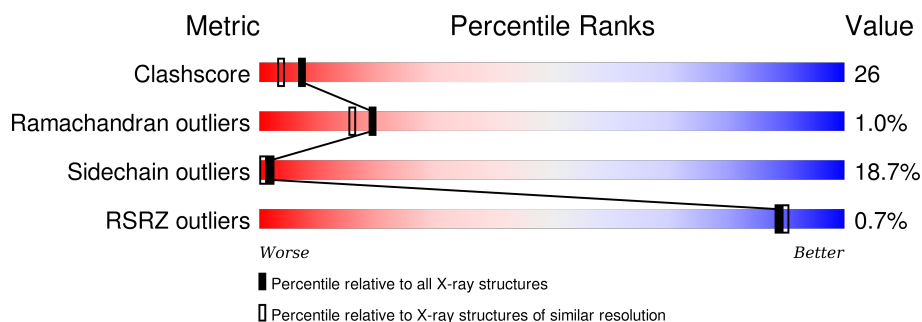
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.25 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))
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	437	
1	B	437	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7101 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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3402	2173	585	628	16			
1	B	434	Total	C	N	O	S	0	0	0
			3385	2164	582	623	16			

There are 52 discrepancies between the modelled and reference sequences:

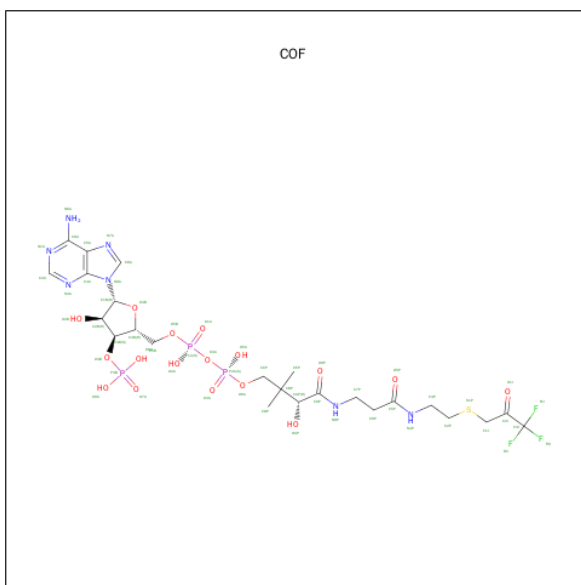
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	ALA	CONFLICT	UNP P23007
A	30	ASN	GLY	CONFLICT	UNP P23007
A	33	VAL	LEU	CONFLICT	UNP P23007
A	52	ILE	VAL	CONFLICT	UNP P23007
A	81	ALA	-	INSERTION	UNP P23007
A	85	GLU	GLY	CONFLICT	UNP P23007
A	104	PRO	GLY	CONFLICT	UNP P23007
A	105	GLU	ALA	CONFLICT	UNP P23007
A	110	VAL	LEU	CONFLICT	UNP P23007
A	163	ASN	LEU	CONFLICT	UNP P23007
A	170	PHE	MET	CONFLICT	UNP P23007
A	174	ASP	SER	CONFLICT	UNP P23007
A	222	PRO	ALA	CONFLICT	UNP P23007
A	283	LEU	GLY	CONFLICT	UNP P23007
A	286	SER	ALA	CONFLICT	UNP P23007
A	291	ASP	ALA	CONFLICT	UNP P23007
A	292	LEU	ALA	CONFLICT	UNP P23007
A	298	ASP	-	INSERTION	UNP P23007
A	299	GLU	-	INSERTION	UNP P23007
A	300	LYS	-	INSERTION	UNP P23007
A	343	SER	GLY	CONFLICT	UNP P23007
A	366	LYS	ALA	CONFLICT	UNP P23007
A	368	LYS	ALA	CONFLICT	UNP P23007
A	428	ALA	ASP	CONFLICT	UNP P23007
A	431	GLU	ILE	CONFLICT	UNP P23007

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	LYS	ALA	CONFLICT	UNP P23007
B	12	SER	ALA	CONFLICT	UNP P23007
B	30	ASN	GLY	CONFLICT	UNP P23007
B	33	VAL	LEU	CONFLICT	UNP P23007
B	52	ILE	VAL	CONFLICT	UNP P23007
B	81	ALA	-	INSERTION	UNP P23007
B	85	GLU	GLY	CONFLICT	UNP P23007
B	104	PRO	GLY	CONFLICT	UNP P23007
B	105	GLU	ALA	CONFLICT	UNP P23007
B	110	VAL	LEU	CONFLICT	UNP P23007
B	163	ASN	LEU	CONFLICT	UNP P23007
B	170	PHE	MET	CONFLICT	UNP P23007
B	174	ASP	SER	CONFLICT	UNP P23007
B	222	PRO	ALA	CONFLICT	UNP P23007
B	283	LEU	GLY	CONFLICT	UNP P23007
B	286	SER	ALA	CONFLICT	UNP P23007
B	291	ASP	ALA	CONFLICT	UNP P23007
B	292	LEU	ALA	CONFLICT	UNP P23007
B	298	ASP	-	INSERTION	UNP P23007
B	299	GLU	-	INSERTION	UNP P23007
B	300	LYS	-	INSERTION	UNP P23007
B	343	SER	GLY	CONFLICT	UNP P23007
B	366	LYS	ALA	CONFLICT	UNP P23007
B	368	LYS	ALA	CONFLICT	UNP P23007
B	428	ALA	ASP	CONFLICT	UNP P23007
B	431	GLU	ILE	CONFLICT	UNP P23007
B	432	LYS	ALA	CONFLICT	UNP P23007

- Molecule 2 is TRIFLUOROACETONYL COENZYME A (three-letter code: COF) (formula: $C_{24}H_{37}F_3N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	S	0	1
			71	32	6	9	19	3	2		
2	B	1	Total	C	F	N	O	P	S	0	1
			71	32	6	9	19	3	2		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



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

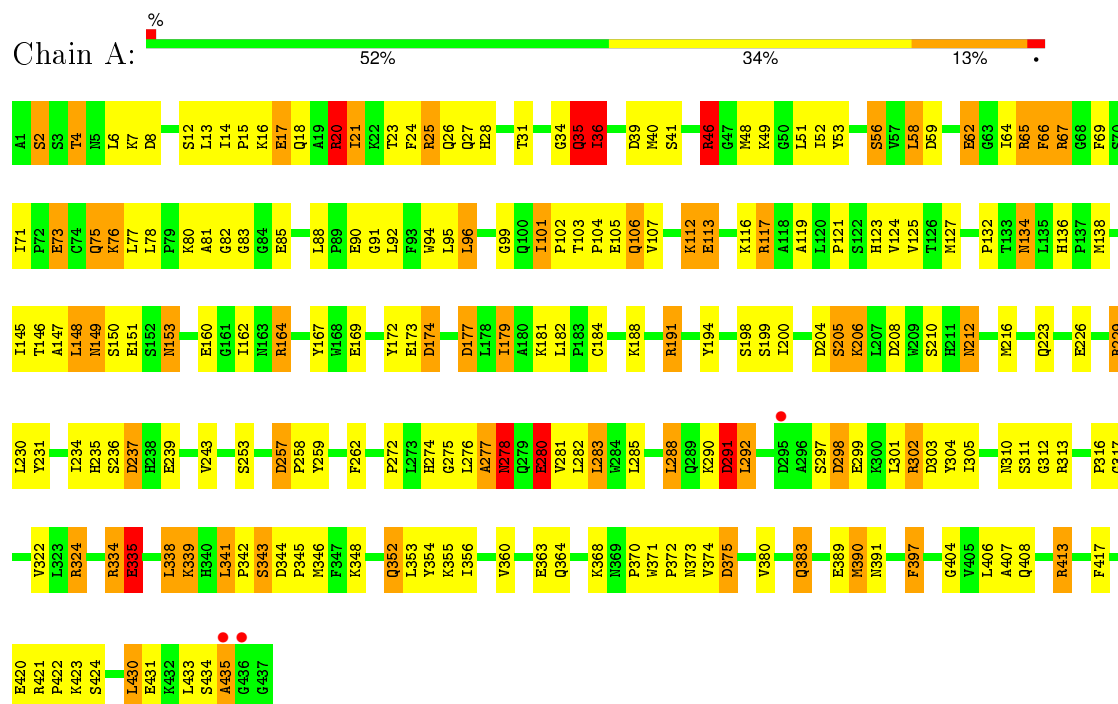
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	0	0
4	B	74	Total 74	O 74	0	0

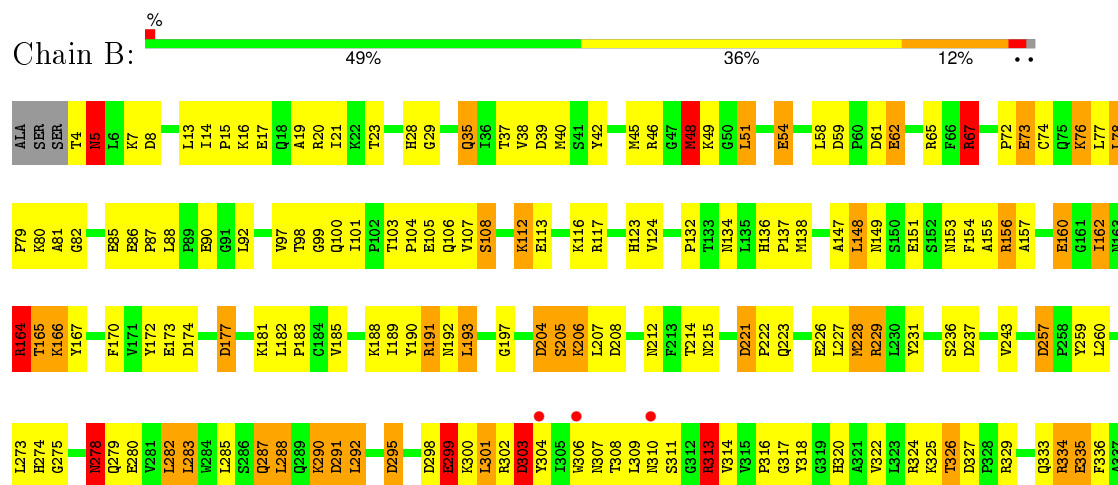
3 Residue-property plots

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: CITRATE SYNTHASE



• Molecule 1: CITRATE SYNTHASE



F417	E420	E421	L430	E431	K432	L433	S434	A435	G436	G437	L338	K339	H340	L341	P342	S343	D344	P345	K346	F347	K348	L349	Q352	L353	Y354	K355	L356	P357	P358	N359	V360	L361	L362	E363	Q364	K368	N369	P370	W371	P372	N373	V374	D375	A376	H377	S378	G379	V380	L381	L382	Q383	T388	E389	M390	N391	F397	R401	G404	A407	Q408	L409	P412
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.37Å 100.21Å 87.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.25 34.54 – 2.23	Depositor EDS
% Data completeness (in resolution range)	86.0 (25.00-2.25) 84.1 (34.54-2.23)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.22Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, R_{free}	0.158 , (Not available) 0.148 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 110.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 40588 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7101	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: COF, 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	1.01	21/3487 (0.6%)	1.36	46/4736 (1.0%)
1	B	0.97	18/3470 (0.5%)	1.41	49/4713 (1.0%)
All	All	0.99	39/6957 (0.6%)	1.39	95/9449 (1.0%)

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	1	0
1	B	1	0
All	All	2	0

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	GLU	CD-OE1	8.07	1.34	1.25
1	A	90	GLU	CD-OE2	7.66	1.34	1.25
1	B	335	GLU	CD-OE1	7.18	1.33	1.25
1	B	90	GLU	CD-OE2	6.86	1.33	1.25
1	A	151	GLU	CD-OE2	6.80	1.33	1.25

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	ARG	NE-CZ-NH1	16.28	128.44	120.30
1	B	229	ARG	NE-CZ-NH2	-12.35	114.12	120.30
1	B	117	ARG	NE-CZ-NH1	10.77	125.69	120.30
1	B	174	ASP	CB-CG-OD2	-10.67	108.70	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	401	ARG	NE-CZ-NH1	10.21	125.41	120.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	THR	CA
1	B	5	ASN	CA

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	3402	0	3383	162	0
1	B	3385	0	3365	194	0
2	A	71	0	24	9	0
2	B	71	0	24	17	0
3	A	13	0	5	2	0
3	B	13	0	5	2	0
4	A	72	0	0	4	0
4	B	74	0	0	5	0
All	All	7101	0	6806	359	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 26.

The worst 5 of 359 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:314:VAL:HG21	2:B:700[A]:COF:H72	1.34	1.09
1:B:124:VAL:HG21	1:B:148:LEU:HD13	1.40	1.02
1:A:124:VAL:HG21	1:A:148:LEU:HD13	1.40	1.02
1:A:24:PHE:HA	1:B:437:GLY:HA3	1.44	0.99
1:B:136:HIS:HD2	1:B:138:MET:H	1.10	0.98

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	435/437 (100%)	411 (94%)	19 (4%)	5 (1%)	17	13
1	B	432/437 (99%)	410 (95%)	18 (4%)	4 (1%)	21	18
All	All	867/874 (99%)	821 (95%)	37 (4%)	9 (1%)	19	16

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	36	ILE
1	A	435	ALA
1	B	311	SER
1	B	435	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	362/362 (100%)	295 (82%)	67 (18%)	2	1
1	B	360/362 (99%)	292 (81%)	68 (19%)	2	0
All	All	722/724 (100%)	587 (81%)	135 (19%)	2	0

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	PHE
1	B	51	LEU
1	B	368	LYS
1	A	413	ARG
1	B	13	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	5	ASN
1	B	100	GLN
1	B	383	GLN
1	B	18	GLN
1	B	26	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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	COF	A	700[A]	-	46,57,57	1.42	6 (13%)	60,86,86	1.52	9 (15%)
2	COF	A	700[B]	-	46,57,57	1.19	3 (6%)	60,86,86	1.30	7 (11%)
3	CIT	A	701	-	3,12,12	1.34	0	3,17,17	1.98	1 (33%)
2	COF	B	700[A]	-	46,57,57	1.26	5 (10%)	60,86,86	1.56	6 (10%)
2	COF	B	700[B]	-	46,57,57	1.08	3 (6%)	60,86,86	1.57	8 (13%)
3	CIT	B	701	-	3,12,12	0.88	0	3,17,17	2.24	1 (33%)

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	COF	A	700[A]	-	-	0/53/74/74	0/3/3/3
2	COF	A	700[B]	-	-	0/53/74/74	0/3/3/3
3	CIT	A	701	-	-	0/6/16/16	0/0/0/0
2	COF	B	700[A]	-	-	0/53/74/74	0/3/3/3
2	COF	B	700[B]	-	-	0/53/74/74	0/3/3/3
3	CIT	B	701	-	-	0/6/16/16	0/0/0/0

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700[A]	COF	C9P-N8P	-3.20	1.26	1.33
2	A	700[A]	COF	C7P-N8P	-3.12	1.38	1.46
2	A	700[A]	COF	CDP-CBP	-2.65	1.48	1.53
2	A	700[B]	COF	CDP-CBP	-2.65	1.48	1.53
2	B	700[A]	COF	C7P-N8P	-2.62	1.40	1.46

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700[A]	COF	P2A-O3A-P1A	-6.87	113.44	132.73
2	B	700[B]	COF	P2A-O3A-P1A	-6.87	113.44	132.73
2	A	700[A]	COF	C2B-C1B-N9A	-4.73	107.06	114.29
2	A	700[B]	COF	C2B-C1B-N9A	-4.73	107.06	114.29
3	B	701	CIT	C3-C4-C5	-3.88	108.75	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700[A]	COF	8	0
2	A	700[B]	COF	1	0
3	A	701	CIT	2	0
2	B	700[A]	COF	12	0
2	B	700[B]	COF	5	0
3	B	701	CIT	2	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	437/437 (100%)	-0.75	3 (0%) 89 90	1, 13, 51, 95	0
1	B	434/437 (99%)	-0.67	3 (0%) 89 90	2, 14, 53, 74	0
All	All	871/874 (99%)	-0.71	6 (0%) 89 90	1, 14, 53, 95	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	TRP	6.0
1	A	436	GLY	3.6
1	A	435	ALA	3.2
1	B	304	TYR	2.5
1	B	310	ASN	2.5

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	COF	A	700[A]	55/55	0.98	0.10	1.04	1,13,74,100	16
2	COF	A	700[B]	55/55	0.98	0.10	1.04	1,13,81,100	16
2	COF	B	700[A]	55/55	0.96	0.12	0.22	1,23,100,100	16
2	COF	B	700[B]	55/55	0.96	0.12	0.22	1,21,100,100	16
3	CIT	A	701	13/13	0.98	0.09	-0.39	1,4,29,46	0
3	CIT	B	701	13/13	0.99	0.09	-0.48	1,5,26,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.