



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 10:33 AM UTC

PDB ID : 1XF1 / pdb_00001xf1
Title : Structure of C5a peptidase- a key virulence factor from Streptococcus
Authors : Brown, C.K.; Gu, Z.Y.; Cleary, P.P.; Matsuka, Y.; Olmstead, S.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on : 2004-09-13
Resolution : 1.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

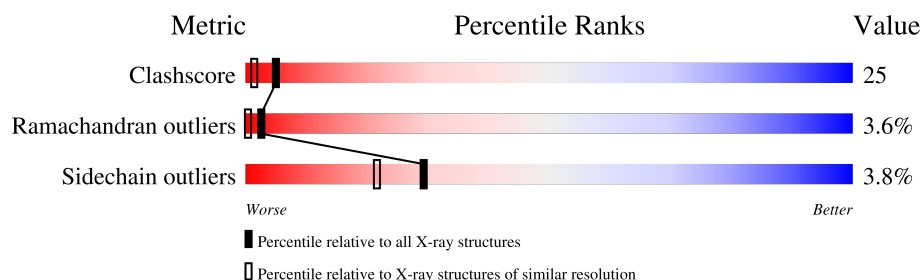
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	926	 65% 29% 5%
1	B	926	 58% 36% 6%

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
4	CIT	A	1101	-	X	-	-
4	CIT	A	1103	-	X	-	-
4	CIT	B	1102	-	X	-	-
4	CIT	B	1104	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	B	1106	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15509 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 C5a peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	926	Total	C	N	O	Se	0	0	0
			7182	4510	1211	1445	16			
1	B	926	Total	C	N	O	Se	4	0	0
			7182	4510	1211	1445	16			

There are 38 discrepancies between the modelled and reference sequences:

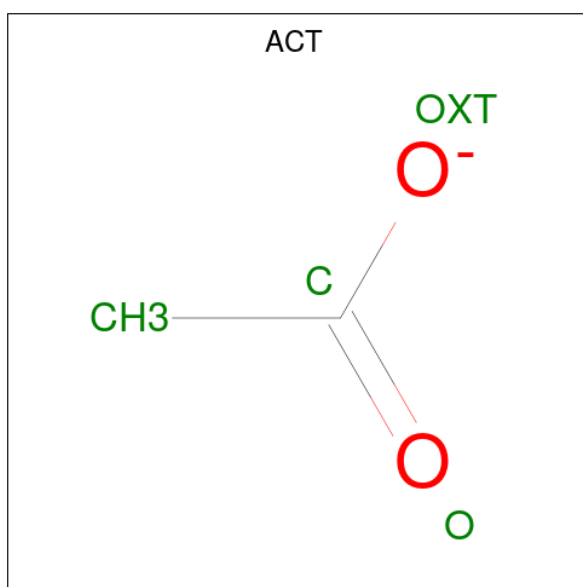
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MSE	MET	modified residue	UNP P15926
A	227	MSE	MET	modified residue	UNP P15926
A	259	MSE	MET	modified residue	UNP P15926
A	353	MSE	MET	modified residue	UNP P15926
A	433	MSE	MET	modified residue	UNP P15926
A	513	MSE	MET	modified residue	UNP P15926
A	522	MSE	MET	modified residue	UNP P15926
A	536	MSE	MET	modified residue	UNP P15926
A	550	MSE	MET	modified residue	UNP P15926
A	585	MSE	MET	modified residue	UNP P15926
A	648	THR	ALA	SEE REMARK 999	UNP P15926
A	680	MSE	MET	modified residue	UNP P15926
A	697	THR	LYS	SEE REMARK 999	UNP P15926
A	702	MSE	MET	modified residue	UNP P15926
A	794	PHE	LEU	SEE REMARK 999	UNP P15926
A	969	MSE	MET	modified residue	UNP P15926
A	996	MSE	THR	engineered mutation	UNP P15926
A	1005	MSE	MET	modified residue	UNP P15926
A	1015	MSE	MET	modified residue	UNP P15926
B	219	MSE	MET	modified residue	UNP P15926
B	227	MSE	MET	modified residue	UNP P15926
B	259	MSE	MET	modified residue	UNP P15926
B	353	MSE	MET	modified residue	UNP P15926
B	433	MSE	MET	modified residue	UNP P15926
B	513	MSE	MET	modified residue	UNP P15926

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Chain	Residue	Modelled	Actual	Comment	Reference
B	522	MSE	MET	modified residue	UNP P15926
B	536	MSE	MET	modified residue	UNP P15926
B	550	MSE	MET	modified residue	UNP P15926
B	585	MSE	MET	modified residue	UNP P15926
B	648	THR	ALA	SEE REMARK 999	UNP P15926
B	680	MSE	MET	modified residue	UNP P15926
B	697	THR	LYS	SEE REMARK 999	UNP P15926
B	702	MSE	MET	modified residue	UNP P15926
B	794	PHE	LEU	SEE REMARK 999	UNP P15926
B	969	MSE	MET	modified residue	UNP P15926
B	996	MSE	THR	engineered mutation	UNP P15926
B	1005	MSE	MET	modified residue	UNP P15926
B	1015	MSE	MET	modified residue	UNP P15926

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

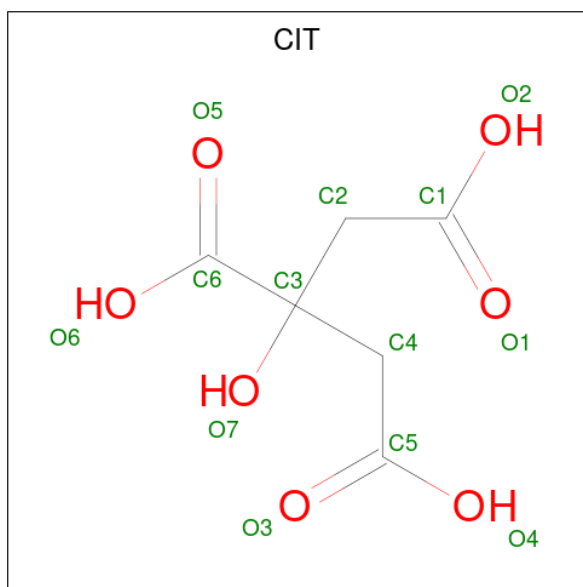


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



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

- Molecule 5 is water.

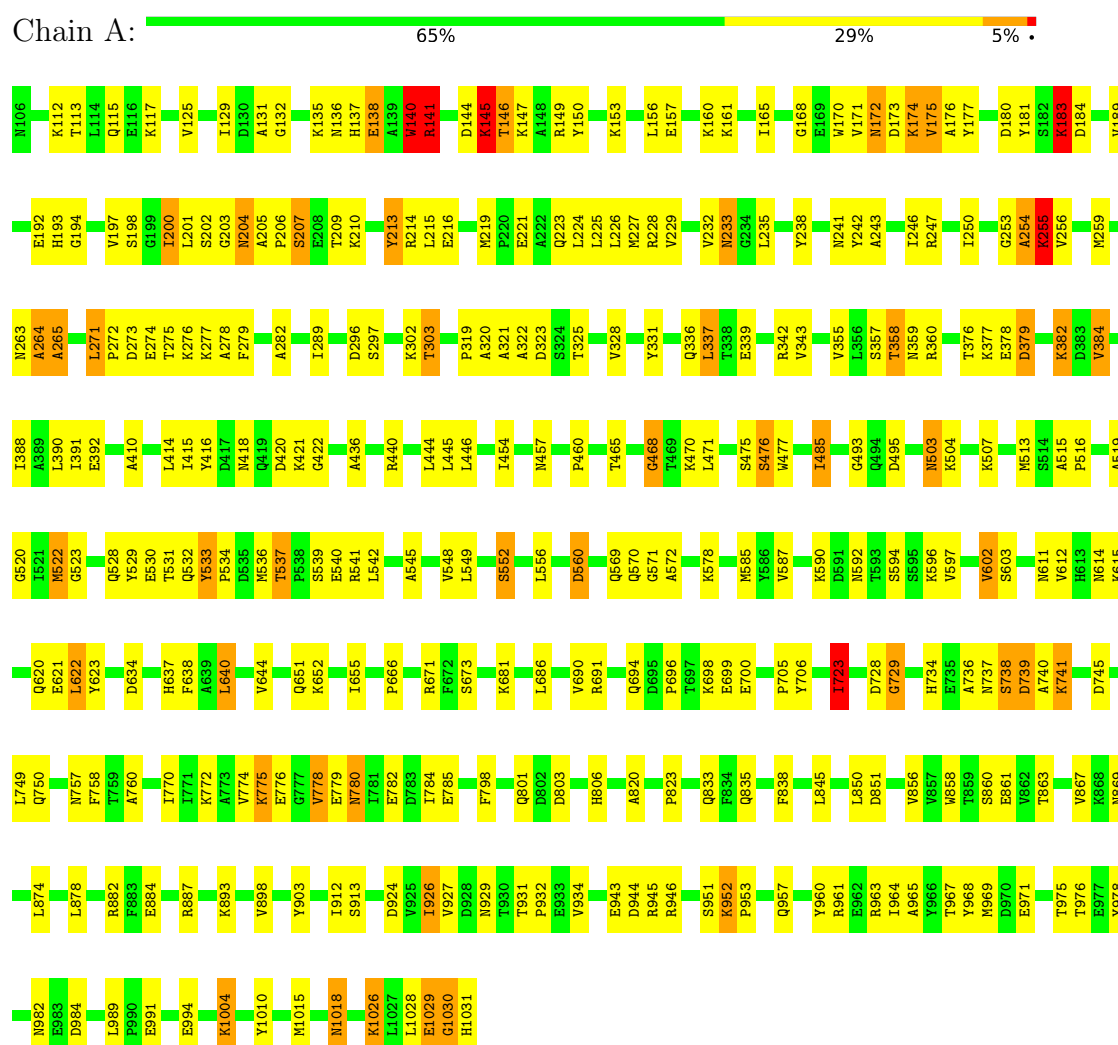
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	544	Total O 544 544	0	0
5	B	513	Total O 513 513	0	0

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: C5a peptidase



• Molecule 1: C5a peptidase



M969	N106	H179	L252	T358	F437	E530	L622	N737	K852
L973	D107	D160	G253	M359	I438	T531	Y623	S738	K858
P974	P108	Y181	A254	R360	S439	Q532	A626	D739	V858
Y978	S109	G185	K255	F361	R440	Y533	L640	K741	T859
D984	Q110	K186	V256	E362	K441	D442	F638	D742	S860
E991	V111	V189	M259	P363	L445	L446	A639	Q743	E861
E994	K112	G190	N263	N364	L445	L446	L640	E744	V862
T995	E116	Q191	A264	K365	N449	N450	V644	D745	N869
M996	G123	G194	A265	A366	Q451	Q452	Q651	L749	L874
E997	T124	H196	L266	Y367	K452	K453	K652	N757	L878
G998	V125	V197	N270	D368	T453	T454	T653	F758	T759
A999	V126	S198	L271	Y369	T455	T456	T654	A760	R882
Y1010	A127	G199	L275	A370	F456	N457	A657	K772	F883
D1014	V128	I200	E274	Y371	N457	T554	K658	K775	E884
M1015	F133	L201	T275	A372	P460	A555	S659	E776	K885
N1018	D134	S202	F279	N373	V462	L556	Q662	G777	T886
I1019	K135	P206	K283	A389	T465	Y557	V663	V778	R887
T1020	K136	E208	V287	L390	Q468	K562	T664	E779	V888
K1026	E137	T209	S297	I391	L471	P567	V665	N780	K893
E1029	E138	K210	I388	E392	S475	Q570	F666	I781	D894
G1030	T146	E216	L337	D397	W477	A572	I667	E782	V898
H1031	K147	G217	T338	F398	I485	M585	R671	D783	Y903
	A148	A218	E339	K406	K486	K590	Q694	E784	T910
	R149	M219	V340	K407	P492	D589	D695	E785	P911
	Q151	P220	V341	A408	Q493	D591	K698	S786	T912
	S152	E221	R342	G409	D495	T593	F699	S787	S913
	K153	Q223	K344	A410	I496	K596	E700	F796	P932
	D155	L225	T345	V411	V500	N601	T704	F798	E933
	L156	L226	A346	G412	N503	F606	Y706	Q801	F940
	E157	M227	T345	V413	K504	T609	I707	D804	S941
	K158	R228	K344	L414	M513	V610	F713	S805	T942
	A159	V229	T345	I415	A515	N611	T723	H806	E943
	K160	E230	A346	Y416	P516	M614	Y724	I809	D944
	R161	I231	D347	Q419	M522	N614	Y724	Y818	R945
	E162	V232	Q348	A425	L524	S616	G729	S822	R946
	Y167	N233	M353	E426	L524	D617	Q729	R829	K952
	G168	A236	P354	L427	L524	K618	A736	Q833	P953
	E169	A236	P354	L427	L524	K618	A736	F834	V959
	W170	R240	V355	E426	L524	K618	A736	Q835	Y960
	N171	Y242	L356	L427	L524	K618	A736	R961	R961
	D173	Y242	L356	L427	L524	K618	A736	F838	E962
	K174	I246	A176	L427	L524	K618	A736	N844	R963
	V175	R247	A176	L427	L524	K618	A736	E735	I964
	A177	D248	S357	L427	L524	K618	A736	E735	A965
	Y178			L427	L524	K618	A736	E735	

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.70Å 75.11Å 132.39Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

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: ACT, CA, 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	0.38	0/7312	0.90	37/9884 (0.4%)
1	B	0.37	0/7312	0.89	23/9884 (0.2%)
All	All	0.38	0/14624	0.90	60/19768 (0.3%)

There are no bond length outliers.

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	TRP	N-CA-C	-8.98	101.90	112.86
1	A	265	ALA	N-CA-C	-7.78	101.96	113.40
1	A	729	GLY	N-CA-C	-7.49	104.71	115.27
1	B	861	GLU	N-CA-C	-7.21	100.81	110.55
1	A	339	GLU	N-CA-C	-7.08	101.19	110.53

There are no chirality outliers.

There are no planarity outliers.

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	7182	0	7004	327	0
1	B	7182	0	7005	400	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	39	0	15	0	0
4	B	39	0	15	2	0
5	A	544	0	0	34	0
5	B	513	0	0	23	0
All	All	15509	0	14045	712	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 25.

The worst 5 of 712 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:778:VAL:HG21	1:A:784:ILE:HD11	1.40	1.03
1:A:210:LYS:HA	1:A:337:LEU:HD12	1.40	1.03
1:B:343:VAL:HG12	1:B:454:ILE:HG22	1.41	1.02
1:A:465:THR:HG23	1:A:468:GLY:H	1.23	1.01
1:B:465:THR:HG23	1:B:468:GLY:H	1.25	1.00

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	924/926 (100%)	830 (90%)	64 (7%)	30 (3%)	3	0
1	B	924/926 (100%)	818 (88%)	70 (8%)	36 (4%)	2	0
All	All	1848/1852 (100%)	1648 (89%)	134 (7%)	66 (4%)	2	0

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	140	TRP
1	A	145	LYS
1	A	172	ASN
1	A	184	ASP

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	771/760 (101%)	742 (96%)	29 (4%)	29	21
1	B	771/760 (101%)	741 (96%)	30 (4%)	28	21
All	All	1542/1520 (101%)	1483 (96%)	59 (4%)	29	21

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1026	LYS
1	B	862	VAL
1	B	246	ILE
1	B	822	SER
1	B	640	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	614	ASN
1	B	869	ASN
1	B	651	GLN
1	B	780	ASN
1	A	757	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	B	1104	-	12,12,12	4.30	4 (33%)	17,17,17	5.71	10 (58%)
4	CIT	B	1106	-	12,12,12	4.24	5 (41%)	17,17,17	5.65	11 (64%)
2	ACT	A	1107	-	3,3,3	0.60	0	3,3,3	0.33	0
4	CIT	A	1105	-	12,12,12	4.45	5 (41%)	17,17,17	5.62	9 (52%)
4	CIT	B	1102	-	12,12,12	4.39	5 (41%)	17,17,17	5.66	11 (64%)
2	ACT	B	1108	-	3,3,3	0.58	0	3,3,3	0.36	0
4	CIT	A	1103	-	12,12,12	4.31	5 (41%)	17,17,17	5.76	10 (58%)
4	CIT	A	1101	-	12,12,12	4.55	5 (41%)	17,17,17	5.70	11 (64%)

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	B	1104	-	-	6/16/16/16	-
4	CIT	B	1106	-	-	4/16/16/16	-
4	CIT	B	1102	-	-	6/16/16/16	-
4	CIT	A	1105	-	-	3/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	A	1103	-	-	6/16/16/16	-
4	CIT	A	1101	-	-	5/16/16/16	-

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	CIT	C3-C6	14.20	1.68	1.53
4	A	1105	CIT	C3-C6	13.74	1.67	1.53
4	B	1102	CIT	C3-C6	13.67	1.67	1.53
4	A	1103	CIT	C3-C6	13.19	1.67	1.53
4	B	1104	CIT	C3-C6	13.07	1.67	1.53

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	CIT	O7-C3-C6	-15.42	87.09	108.96
4	B	1104	CIT	O7-C3-C6	-14.94	87.77	108.96
4	A	1101	CIT	O7-C3-C6	-14.11	88.95	108.96
4	A	1105	CIT	O7-C3-C6	-14.04	89.05	108.96
4	B	1102	CIT	O7-C3-C6	-13.96	89.16	108.96

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	CIT	C1-C2-C3-O7
4	A	1101	CIT	O7-C3-C4-C5
4	A	1103	CIT	C1-C2-C3-O7
4	A	1105	CIT	C1-C2-C3-O7
4	A	1105	CIT	C2-C3-C4-C5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1104	CIT	1	0
4	B	1106	CIT	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.