



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:49 PM UTC

PDB ID : 6TC0 / pdb_00006tc0
Title : Crystal structure of MMS19-CIAO1-CIAO2B CIA targeting complex
Authors : Kassube, S.A.; Thoma, N.H.
Deposited on : 2019-11-04
Resolution : 3.60 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
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

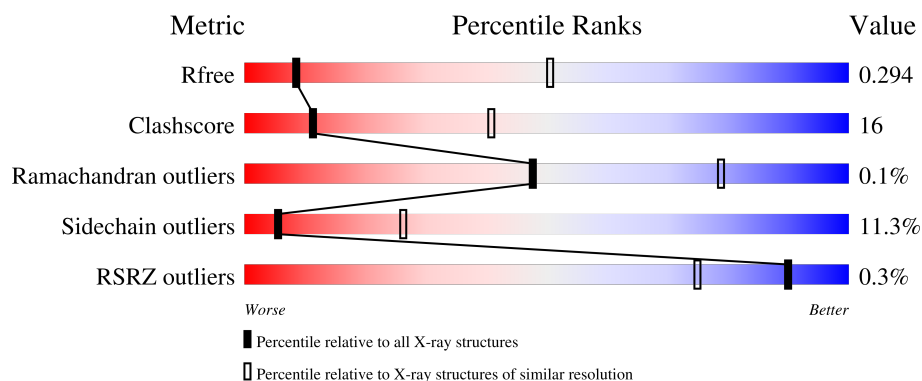
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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 $\leq 5\%$. 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	338	 82% 17% ..
1	D	338	 82% 17% ..
2	B	159	 70% 24% . .
2	E	159	 77% 18% . .
3	C	1035	 57% 33% 6% .

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Mol	Chain	Length	Quality of chain
3	F	1035	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (58%), yellow (31%), and orange (6%). A small black dot is at the end of the bar.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22972 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 Probable cytosolic iron-sulfur protein assembly protein Ciao1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2613	1629	455	516	13			
1	D	336	Total	C	N	O	S	0	0	0
			2613	1629	455	516	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q7K1Y4
A	-1	GLY	-	expression tag	UNP Q7K1Y4
A	0	GLY	-	expression tag	UNP Q7K1Y4
A	1	ARG	-	expression tag	UNP Q7K1Y4
D	-2	GLY	-	expression tag	UNP Q7K1Y4
D	-1	GLY	-	expression tag	UNP Q7K1Y4
D	0	GLY	-	expression tag	UNP Q7K1Y4
D	1	ARG	-	expression tag	UNP Q7K1Y4

- Molecule 2 is a protein called MIP18 family protein galla-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	154	Total	C	N	O	S	0	0	0
			1223	765	217	238	3			
2	E	154	Total	C	N	O	S	0	0	0
			1223	765	217	238	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9VTC4
B	-1	GLY	-	expression tag	UNP Q9VTC4
B	0	GLY	-	expression tag	UNP Q9VTC4
B	1	ARG	-	expression tag	UNP Q9VTC4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP Q9VTC4
E	-1	GLY	-	expression tag	UNP Q9VTC4
E	0	GLY	-	expression tag	UNP Q9VTC4
E	1	ARG	-	expression tag	UNP Q9VTC4

- Molecule 3 is a protein called MMS19 nucleotide excision repair protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	994	Total	C	N	O	S	0	0	0
			7669	4888	1311	1424	46			
3	F	989	Total	C	N	O	S	0	0	0
			7631	4862	1306	1418	45			

There are 8 discrepancies between the modelled and reference sequences:

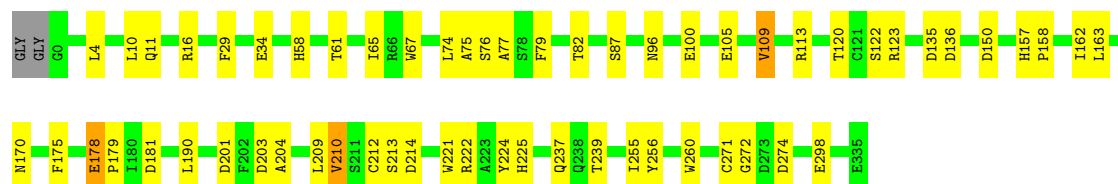
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP Q9D071
C	-2	GLY	-	expression tag	UNP Q9D071
C	-1	GLY	-	expression tag	UNP Q9D071
C	0	ARG	-	expression tag	UNP Q9D071
F	-3	GLY	-	expression tag	UNP Q9D071
F	-2	GLY	-	expression tag	UNP Q9D071
F	-1	GLY	-	expression tag	UNP Q9D071
F	0	ARG	-	expression tag	UNP Q9D071

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.

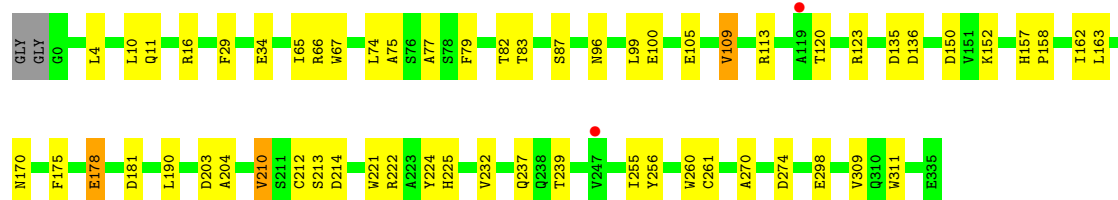
- Molecule 1: Probable cytosolic iron-sulfur protein assembly protein Ciaol

Chain A: 



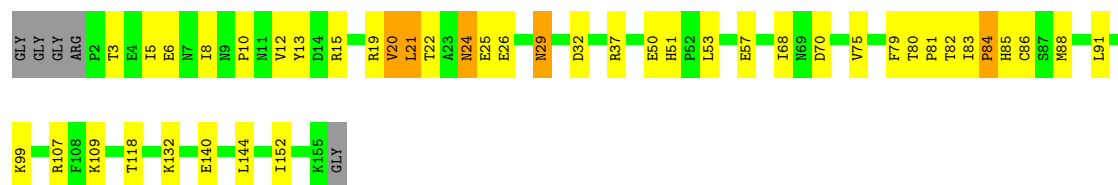
- Molecule 1: Probable cytosolic iron-sulfur protein assembly protein Ciaol

Chain D: 



- Molecule 2: MIP18 family protein galla-2

Chain B: 



- Molecule 2: MIP18 family protein galla-2

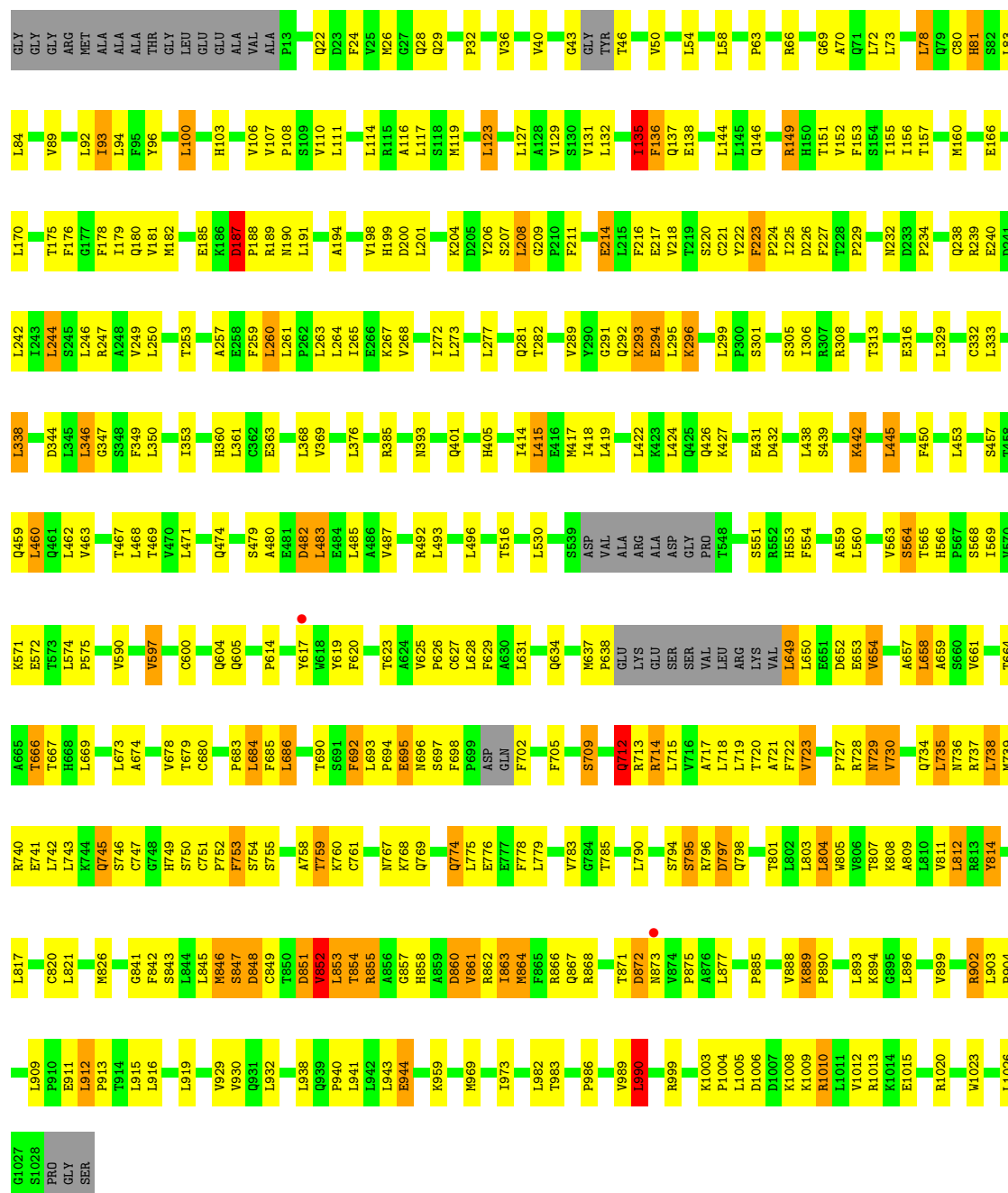
Chain E: 



GLY

• Molecule 3: MMS19 nucleotide excision repair protein homolog

Chain C:  57% 33% 6% .



• Molecule 3: MMS19 nucleotide excision repair protein homolog

Chain F:  58% 31% 6% .

L938	Q939	P940	L941	L942	L943	E944	K959	V969	I973	L982	T983	P986	V989	L990	R999	K1003	P1004	L1005	D1006	D1007	K1008	K1009	R1010	L1011	V1012	R1013	K1014	E1015	R1020	L1026	G1027	S1028	PRO	GLY	SER																	
T679	C751	R852	L853	T854	R855	A856	G857	H858	A859	D860	V861	R862	I863	M864	F865	R866	R867	R868	F869	F870	T871	D872	N873	V874	P875	A876	L877	P885	V888	K889	P890	L893	K894	G895	L896	V899	L900	N901	R902	L903	P904	L909	P910	E911	L912	P913	T914	L915	L916	L919	V929	L932
M589	C751	R852	L853	T854	R855	A856	G857	H858	A859	D860	V861	R862	I863	M864	F865	R866	R867	R868	F869	F870	T871	D872	N873	V874	P875	A876	L877	P885	V888	K889	P890	L893	K894	G895	L896	V899	L900	N901	R902	L903	P904	L909	P910	E911	L912	P913	T914	L915	L916	L919	V929	L932
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
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M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
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M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
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M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640	L649	L650	D651	D652	E653	V654	L655	L658	A659	I662	T666	T667	H668	L669	L673	A674	A675	V678												
L468	T469	L470	L471	G472	A473	Q474	P475	L476	L477	L478	S479	A480	E481	D482	L483	E484	L485	R492	L493	T494	F495	L496	L508	S539	ASP	VAL	ALA	ARG	Q426	K427	E431	D432	R433	D434	S551	R552	H553	F554	L560	S564	T565	H566	P567	S568	I569	V570	K571	E572	L573	L574	P575	A584
M589	V590	Q605	P614	Y617	W618	F619	F620	T623	A624	V625	P626	C627	L628	F629	A630	A632	V633	Q634	M637	P638	L639	L640																														

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.40Å 140.70Å 327.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.60 20.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.60) 99.3 (20.00-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.62Å)	Xtriage
Refinement program	CNS, PHENIX 1.16_3549	Depositor
R, R_{free}	0.258 , 0.277 0.278 , 0.294	Depositor DCC
R_{free} test set	2900 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	175.8	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 120.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22972	wwPDB-VP
Average B, all atoms (Å ²)	211.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/2679	0.64	0/3649
1	D	0.40	0/2679	0.68	0/3649
2	B	0.55	0/1244	1.06	11/1694 (0.6%)
2	E	0.49	0/1244	0.92	6/1694 (0.4%)
3	C	0.42	1/7816 (0.0%)	0.79	14/10614 (0.1%)
3	F	0.44	1/7775 (0.0%)	0.78	6/10558 (0.1%)
All	All	0.43	2/23437 (0.0%)	0.78	37/31858 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	682	VAL	CA-CB	-8.03	1.50	1.54
3	C	187	ASP	CB-CG	-5.26	1.38	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	TYR	CA-C-N	11.02	135.05	120.28
2	B	13	TYR	C-N-CA	11.02	135.05	120.28
2	E	10	PRO	CA-C-N	9.60	134.10	120.28
2	E	10	PRO	C-N-CA	9.60	134.10	120.28
2	B	3	THR	CA-C-N	7.55	132.15	120.75

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	2613	0	2480	39	0
1	D	2613	0	2480	33	0
2	B	1223	0	1230	56	0
2	E	1223	0	1230	41	0
3	C	7669	0	7810	311	0
3	F	7631	0	7774	316	0
All	All	22972	0	23004	743	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 16.

The worst 5 of 743 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)
3:F:226:ASP:HB3	3:F:239:ARG:HD3	1.20	1.19
3:C:226:ASP:HB2	3:C:239:ARG:HD2	1.21	1.12
3:F:751:CYS:SG	3:F:754:SER:N	2.26	1.09
3:F:769:GLN:O	3:F:813:ARG:NH2	1.83	1.09
3:F:474:GLN:H	3:F:474:GLN:CD	1.64	1.01

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	334/338 (99%)	320 (96%)	14 (4%)	0	100	100
1	D	334/338 (99%)	322 (96%)	12 (4%)	0	100	100
2	B	152/159 (96%)	148 (97%)	4 (3%)	0	100	100
2	E	152/159 (96%)	148 (97%)	4 (3%)	0	100	100
3	C	984/1035 (95%)	936 (95%)	47 (5%)	1 (0%)	48	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	979/1035 (95%)	930 (95%)	48 (5%)	1 (0%)	48 79
All	All	2935/3064 (96%)	2804 (96%)	129 (4%)	2 (0%)	48 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	223	PHE
3	F	223	PHE

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	284/284 (100%)	279 (98%)	5 (2%)	51 68
1	D	284/284 (100%)	279 (98%)	5 (2%)	51 68
2	B	141/142 (99%)	139 (99%)	2 (1%)	59 71
2	E	141/142 (99%)	141 (100%)	0	100 100
3	C	859/887 (97%)	725 (84%)	134 (16%)	2 16
3	F	854/887 (96%)	710 (83%)	144 (17%)	2 13
All	All	2563/2626 (98%)	2273 (89%)	290 (11%)	5 26

5 of 290 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	652	ASP
3	F	990	LEU
3	F	682	VAL
3	F	849	CYS
3	C	753	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	745	GLN
3	F	901	ASN
1	D	310	GLN
3	F	873	ASN
3	F	558	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	336/338 (99%)	-0.64	0 100 100	148, 195, 264, 303	0
1	D	336/338 (99%)	-0.30	2 (0%) 85 64	314, 381, 426, 449	0
2	B	154/159 (96%)	-0.37	0 100 100	164, 192, 281, 306	0
2	E	154/159 (96%)	-0.35	0 100 100	220, 249, 307, 323	0
3	C	994/1035 (96%)	-0.43	2 (0%) 91 80	118, 184, 263, 377	0
3	F	989/1035 (95%)	-0.45	5 (0%) 87 66	111, 167, 234, 375	0
All	All	2963/3064 (96%)	-0.44	9 (0%) 90 75	111, 189, 385, 449	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	873	ASN	5.9
3	F	434	ASP	4.2
1	D	247	VAL	3.5
3	C	617	TYR	3.4
3	F	617	TYR	3.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.