



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:16 AM UTC

PDB ID : 2NVV / pdb_00002nvv
Title : Crystal Structure of the Putative Acetyl-CoA hydrolase/transferase PG1013 from Porphyromonas gingivalis, Northeast Structural Genomics Target PgR16.
Authors : Forouhar, F.; Neely, H.; Seetharaman, J.; Yong, W.; Ho, C.K.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2006-11-13
Resolution : 2.70 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

<https://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)	:	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)

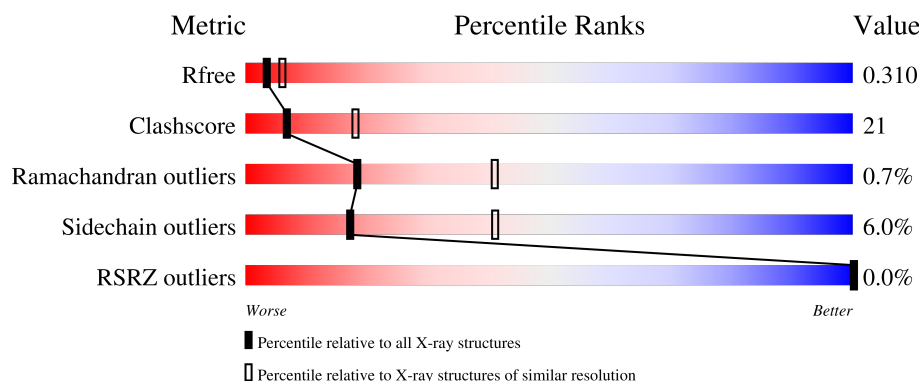
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

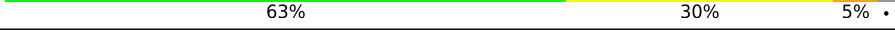
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	506	
1	B	506	
1	C	506	
1	D	506	

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	506	59% 33% 6%
1	F	506	58% 33% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23178 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 Acetyl-CoA hydrolase/transferase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	B	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	C	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	D	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	E	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			
1	F	496	Total	C	N	O	S	Se	0	0	0
			3828	2418	672	720	6	12			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q7MVN7
A	57	MSE	MET	modified residue	UNP Q7MVN7
A	168	MSE	MET	modified residue	UNP Q7MVN7
A	170	MSE	MET	modified residue	UNP Q7MVN7
A	243	MSE	MET	modified residue	UNP Q7MVN7
A	281	MSE	MET	modified residue	UNP Q7MVN7
A	294	MSE	MET	modified residue	UNP Q7MVN7
A	372	MSE	MET	modified residue	UNP Q7MVN7
A	373	MSE	MET	modified residue	UNP Q7MVN7
A	397	MSE	MET	modified residue	UNP Q7MVN7
A	408	MSE	MET	modified residue	UNP Q7MVN7
A	488	MSE	MET	modified residue	UNP Q7MVN7
A	497	MSE	MET	modified residue	UNP Q7MVN7
A	499	LEU	-	expression tag	UNP Q7MVN7
A	500	GLU	-	expression tag	UNP Q7MVN7
A	501	HIS	-	expression tag	UNP Q7MVN7
A	502	HIS	-	expression tag	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	503	HIS	-	expression tag	UNP Q7MVN7
A	504	HIS	-	expression tag	UNP Q7MVN7
A	505	HIS	-	expression tag	UNP Q7MVN7
A	506	HIS	-	expression tag	UNP Q7MVN7
B	1	MSE	MET	modified residue	UNP Q7MVN7
B	57	MSE	MET	modified residue	UNP Q7MVN7
B	168	MSE	MET	modified residue	UNP Q7MVN7
B	170	MSE	MET	modified residue	UNP Q7MVN7
B	243	MSE	MET	modified residue	UNP Q7MVN7
B	281	MSE	MET	modified residue	UNP Q7MVN7
B	294	MSE	MET	modified residue	UNP Q7MVN7
B	372	MSE	MET	modified residue	UNP Q7MVN7
B	373	MSE	MET	modified residue	UNP Q7MVN7
B	397	MSE	MET	modified residue	UNP Q7MVN7
B	408	MSE	MET	modified residue	UNP Q7MVN7
B	488	MSE	MET	modified residue	UNP Q7MVN7
B	497	MSE	MET	modified residue	UNP Q7MVN7
B	499	LEU	-	expression tag	UNP Q7MVN7
B	500	GLU	-	expression tag	UNP Q7MVN7
B	501	HIS	-	expression tag	UNP Q7MVN7
B	502	HIS	-	expression tag	UNP Q7MVN7
B	503	HIS	-	expression tag	UNP Q7MVN7
B	504	HIS	-	expression tag	UNP Q7MVN7
B	505	HIS	-	expression tag	UNP Q7MVN7
B	506	HIS	-	expression tag	UNP Q7MVN7
C	1	MSE	MET	modified residue	UNP Q7MVN7
C	57	MSE	MET	modified residue	UNP Q7MVN7
C	168	MSE	MET	modified residue	UNP Q7MVN7
C	170	MSE	MET	modified residue	UNP Q7MVN7
C	243	MSE	MET	modified residue	UNP Q7MVN7
C	281	MSE	MET	modified residue	UNP Q7MVN7
C	294	MSE	MET	modified residue	UNP Q7MVN7
C	372	MSE	MET	modified residue	UNP Q7MVN7
C	373	MSE	MET	modified residue	UNP Q7MVN7
C	397	MSE	MET	modified residue	UNP Q7MVN7
C	408	MSE	MET	modified residue	UNP Q7MVN7
C	488	MSE	MET	modified residue	UNP Q7MVN7
C	497	MSE	MET	modified residue	UNP Q7MVN7
C	499	LEU	-	expression tag	UNP Q7MVN7
C	500	GLU	-	expression tag	UNP Q7MVN7
C	501	HIS	-	expression tag	UNP Q7MVN7
C	502	HIS	-	expression tag	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	503	HIS	-	expression tag	UNP Q7MVN7
C	504	HIS	-	expression tag	UNP Q7MVN7
C	505	HIS	-	expression tag	UNP Q7MVN7
C	506	HIS	-	expression tag	UNP Q7MVN7
D	1	MSE	MET	modified residue	UNP Q7MVN7
D	57	MSE	MET	modified residue	UNP Q7MVN7
D	168	MSE	MET	modified residue	UNP Q7MVN7
D	170	MSE	MET	modified residue	UNP Q7MVN7
D	243	MSE	MET	modified residue	UNP Q7MVN7
D	281	MSE	MET	modified residue	UNP Q7MVN7
D	294	MSE	MET	modified residue	UNP Q7MVN7
D	372	MSE	MET	modified residue	UNP Q7MVN7
D	373	MSE	MET	modified residue	UNP Q7MVN7
D	397	MSE	MET	modified residue	UNP Q7MVN7
D	408	MSE	MET	modified residue	UNP Q7MVN7
D	488	MSE	MET	modified residue	UNP Q7MVN7
D	497	MSE	MET	modified residue	UNP Q7MVN7
D	499	LEU	-	expression tag	UNP Q7MVN7
D	500	GLU	-	expression tag	UNP Q7MVN7
D	501	HIS	-	expression tag	UNP Q7MVN7
D	502	HIS	-	expression tag	UNP Q7MVN7
D	503	HIS	-	expression tag	UNP Q7MVN7
D	504	HIS	-	expression tag	UNP Q7MVN7
D	505	HIS	-	expression tag	UNP Q7MVN7
D	506	HIS	-	expression tag	UNP Q7MVN7
E	1	MSE	MET	modified residue	UNP Q7MVN7
E	57	MSE	MET	modified residue	UNP Q7MVN7
E	168	MSE	MET	modified residue	UNP Q7MVN7
E	170	MSE	MET	modified residue	UNP Q7MVN7
E	243	MSE	MET	modified residue	UNP Q7MVN7
E	281	MSE	MET	modified residue	UNP Q7MVN7
E	294	MSE	MET	modified residue	UNP Q7MVN7
E	372	MSE	MET	modified residue	UNP Q7MVN7
E	373	MSE	MET	modified residue	UNP Q7MVN7
E	397	MSE	MET	modified residue	UNP Q7MVN7
E	408	MSE	MET	modified residue	UNP Q7MVN7
E	488	MSE	MET	modified residue	UNP Q7MVN7
E	497	MSE	MET	modified residue	UNP Q7MVN7
E	499	LEU	-	expression tag	UNP Q7MVN7
E	500	GLU	-	expression tag	UNP Q7MVN7
E	501	HIS	-	expression tag	UNP Q7MVN7
E	502	HIS	-	expression tag	UNP Q7MVN7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	503	HIS	-	expression tag	UNP Q7MVN7
E	504	HIS	-	expression tag	UNP Q7MVN7
E	505	HIS	-	expression tag	UNP Q7MVN7
E	506	HIS	-	expression tag	UNP Q7MVN7
F	1	MSE	MET	modified residue	UNP Q7MVN7
F	57	MSE	MET	modified residue	UNP Q7MVN7
F	168	MSE	MET	modified residue	UNP Q7MVN7
F	170	MSE	MET	modified residue	UNP Q7MVN7
F	243	MSE	MET	modified residue	UNP Q7MVN7
F	281	MSE	MET	modified residue	UNP Q7MVN7
F	294	MSE	MET	modified residue	UNP Q7MVN7
F	372	MSE	MET	modified residue	UNP Q7MVN7
F	373	MSE	MET	modified residue	UNP Q7MVN7
F	397	MSE	MET	modified residue	UNP Q7MVN7
F	408	MSE	MET	modified residue	UNP Q7MVN7
F	488	MSE	MET	modified residue	UNP Q7MVN7
F	497	MSE	MET	modified residue	UNP Q7MVN7
F	499	LEU	-	expression tag	UNP Q7MVN7
F	500	GLU	-	expression tag	UNP Q7MVN7
F	501	HIS	-	expression tag	UNP Q7MVN7
F	502	HIS	-	expression tag	UNP Q7MVN7
F	503	HIS	-	expression tag	UNP Q7MVN7
F	504	HIS	-	expression tag	UNP Q7MVN7
F	505	HIS	-	expression tag	UNP Q7MVN7
F	506	HIS	-	expression tag	UNP Q7MVN7

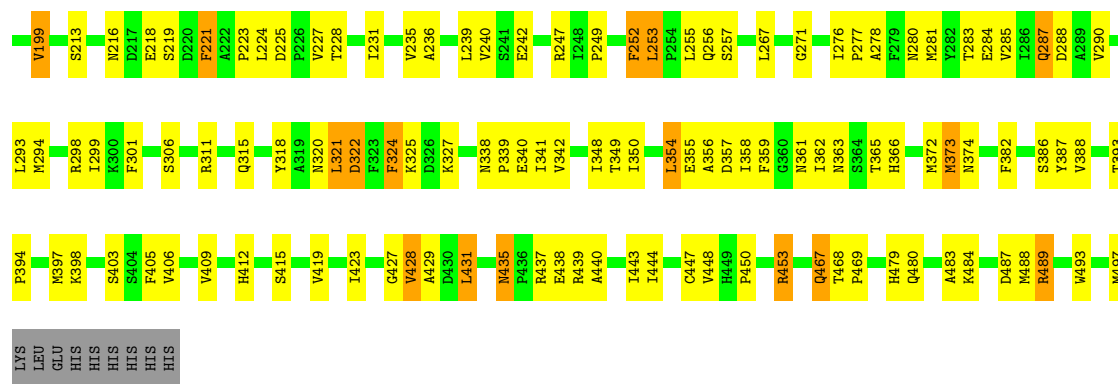
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	2	Total Zn 2 2	0	0

- Molecule 3 is water.

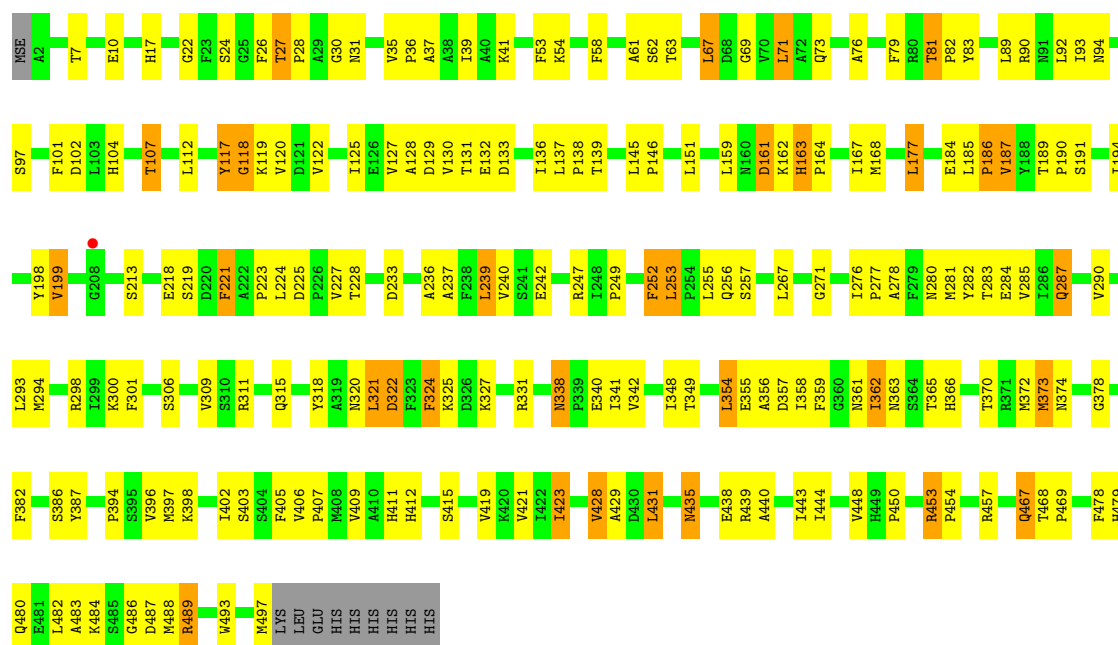
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	22	Total 22	O 22	0	0
3	C	30	Total 30	O 30	0	0
3	D	23	Total 23	O 23	0	0
3	E	52	Total 52	O 52	0	0
3	F	47	Total 47	O 47	0	0

F101	F102	L103	H104	L105	S106	Y117	G118	L119	V120	D121	V122	L125	E126	V127	A128	D129	V130	T131	E132	D133	L136	L137	P138	T139	L145	P146	L151	L159	H160	D161	K162	H163	P164	K165	E166	M167	L168	L173	C174	L177	E184	L185	P186	V187	H188	T189	P190	S191	T194
N5E	A2	T7	A8	E9	E10	H17	G22	F23	S24	G25	F26	T27	A28	G29	G30	V35	P36	A37	K41	K54	F58	A61	S62	T63	L67	D68	G69	V70	L71	A72	Q73	A76	V77	K78	F79	R80	T81	P82	Y83	L89	R90	G93	L92	L93	N94	S97	T104		



● Molecule 1: Acetyl-CoA hydrolase/transferase family protein

Chain F: 58% 33% 6% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	131.05Å 131.05Å 162.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 2.70 19.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.95-2.70) 52.4 (19.95-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.63 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1, XTALVIEW	Depositor
R, R_{free}	0.287 , 0.290 0.306 , 0.310	Depositor DCC
R_{free} test set	8375 reflections (6.88%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 10.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.499 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.012 for H, K, L 0.496 for -H, H+K, -L 0.492 for -h,-k,l	Depositor
Outliers	0 of 121779 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	23178	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.72% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.47	0/3898	1.00	16/5269 (0.3%)
1	B	0.46	0/3898	1.00	15/5269 (0.3%)
1	C	0.48	0/3898	1.00	15/5269 (0.3%)
1	D	0.47	0/3898	1.00	19/5269 (0.4%)
1	E	0.48	0/3898	0.99	13/5269 (0.2%)
1	F	0.48	0/3898	1.00	17/5269 (0.3%)
All	All	0.47	0/23388	1.00	95/31614 (0.3%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	N-CA-C	-6.75	104.00	111.36
1	E	354	LEU	N-CA-C	-6.57	104.20	111.36
1	B	104	HIS	N-CA-C	-6.45	100.10	109.59
1	C	104	HIS	N-CA-C	-6.43	100.13	109.59
1	C	354	LEU	N-CA-C	-6.43	104.36	111.36

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	3828	0	3808	160	0
1	B	3828	0	3808	158	0
1	C	3828	0	3808	155	0
1	D	3828	0	3808	160	0
1	E	3828	0	3808	177	0
1	F	3828	0	3808	195	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
3	A	30	0	0	10	0
3	B	22	0	0	9	0
3	C	30	0	0	2	0
3	D	23	0	0	2	0
3	E	52	0	0	20	0
3	F	47	0	0	30	0
All	All	23178	0	22848	981	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 21.

The worst 5 of 981 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:298:ARG:HB2	3:A:516:HOH:O	1.58	1.03
1:F:419:VAL:HG12	3:F:517:HOH:O	1.67	0.94
1:E:136:ILE:HB	1:E:199:VAL:HG13	1.50	0.93
1:F:136:ILE:HB	1:F:199:VAL:HG13	1.51	0.92
1:A:94:ASN:HD21	1:A:372:MSE:H	1.18	0.91

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	494/506 (98%)	458 (93%)	33 (7%)	3 (1%)	21	44
1	B	494/506 (98%)	462 (94%)	29 (6%)	3 (1%)	21	44
1	C	494/506 (98%)	460 (93%)	31 (6%)	3 (1%)	21	44
1	D	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	16	37
1	E	494/506 (98%)	461 (93%)	29 (6%)	4 (1%)	16	37
1	F	494/506 (98%)	460 (93%)	30 (6%)	4 (1%)	16	37
All	All	2964/3036 (98%)	2762 (93%)	181 (6%)	21 (1%)	18	41

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	A	221	PHE
1	B	118	GLY
1	B	221	PHE
1	C	118	GLY

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	416/413 (101%)	390 (94%)	26 (6%)	16	39
1	B	416/413 (101%)	392 (94%)	24 (6%)	18	42
1	C	416/413 (101%)	391 (94%)	25 (6%)	17	41
1	D	416/413 (101%)	392 (94%)	24 (6%)	18	42
1	E	416/413 (101%)	391 (94%)	25 (6%)	17	41
1	F	416/413 (101%)	391 (94%)	25 (6%)	17	41
All	All	2496/2478 (101%)	2347 (94%)	149 (6%)	17	41

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	321	LEU
1	F	428	VAL
1	E	431	LEU
1	F	161	ASP
1	B	453	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 121 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	458	GLN
1	F	261	ASN
1	D	264	ASN
1	F	200	GLN
1	F	467	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](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å²)	Q<0.9	
1	A	484/506 (95%)	-1.09	0	100	100	6, 7, 18, 30	0
1	B	484/506 (95%)	-1.09	0	100	100	6, 7, 18, 30	0
1	C	484/506 (95%)	-1.08	0	100	100	6, 7, 18, 30	0
1	D	484/506 (95%)	-1.04	0	100	100	6, 7, 18, 30	0
1	E	484/506 (95%)	-0.93	0	100	100	6, 7, 18, 30	0
1	F	484/506 (95%)	-0.91	1 (0%)	91	90	6, 7, 18, 30	0
All	All	2904/3036 (95%)	-1.02	1 (0%)	100	100	6, 7, 18, 30	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	208	GLY	2.4

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](#)

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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	E	508	1/1	0.98	0.05	25,25,25,25	0
2	ZN	C	507	1/1	0.99	0.02	18,18,18,18	0
2	ZN	E	507	1/1	0.99	0.02	15,15,15,15	0
2	ZN	B	507	1/1	0.99	0.02	20,20,20,20	0
2	ZN	A	507	1/1	1.00	0.01	16,16,16,16	0
2	ZN	D	507	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.