



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:39 AM UTC

PDB ID : 9NZ6 / pdb_00009nz6
Title : Oxidoreductase isolated from Xanthomonas citri pv. citri A306
Authors : Santos, L.S.; Torres, S.C.; Balan, A.
Deposited on : 2025-03-31
Resolution : 2.98 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

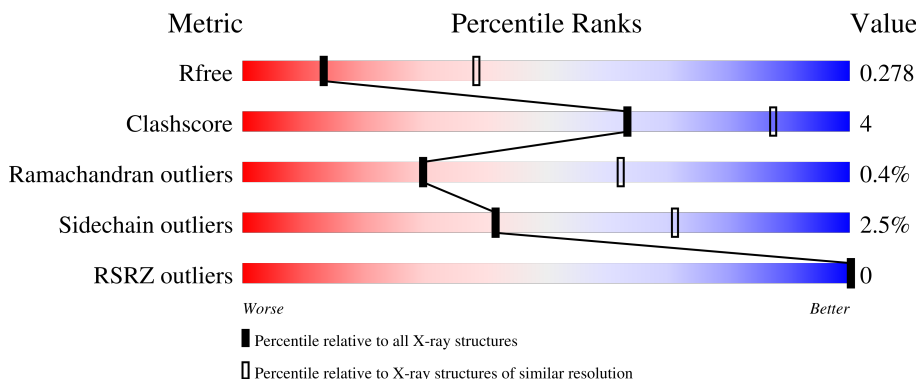
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	365	
1	B	365	
1	C	365	
1	D	365	
1	E	365	

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Mol	Chain	Length	Quality of chain
1	F	365	 68%13%•18%
1	G	365	 70%11%19%
1	H	365	 71%10%•18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19052 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 Oxidoreductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2437	1550	437	448	2			
1	B	313	Total	C	N	O	S	0	0	0
			2446	1555	438	451	2			
1	C	309	Total	C	N	O	S	0	0	0
			2415	1536	432	445	2			
1	D	309	Total	C	N	O	S	0	0	0
			2419	1539	434	444	2			
1	E	298	Total	C	N	O	S	0	0	0
			2320	1477	415	426	2			
1	F	300	Total	C	N	O	S	0	0	0
			2345	1493	422	428	2			
1	G	297	Total	C	N	O	S	0	0	0
			2318	1476	415	425	2			
1	H	301	Total	C	N	O	S	0	0	0
			2349	1495	423	429	2			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP A0AAI7ZHB9
A	-1	GLY	-	expression tag	UNP A0AAI7ZHB9
A	0	SER	-	expression tag	UNP A0AAI7ZHB9
A	1	SER	-	expression tag	UNP A0AAI7ZHB9
A	2	HIS	-	expression tag	UNP A0AAI7ZHB9
A	3	HIS	-	expression tag	UNP A0AAI7ZHB9
A	4	HIS	-	expression tag	UNP A0AAI7ZHB9
A	5	HIS	-	expression tag	UNP A0AAI7ZHB9
A	6	HIS	-	expression tag	UNP A0AAI7ZHB9
A	7	HIS	-	expression tag	UNP A0AAI7ZHB9
A	8	SER	-	expression tag	UNP A0AAI7ZHB9
A	9	SER	-	expression tag	UNP A0AAI7ZHB9
A	10	GLY	-	expression tag	UNP A0AAI7ZHB9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	11	LEU	-	expression tag	UNP A0AAI7ZHB9
A	12	VAL	-	expression tag	UNP A0AAI7ZHB9
A	13	PRO	-	expression tag	UNP A0AAI7ZHB9
A	14	ARG	-	expression tag	UNP A0AAI7ZHB9
A	15	GLY	-	expression tag	UNP A0AAI7ZHB9
A	16	SER	-	expression tag	UNP A0AAI7ZHB9
B	1	MET	-	initiating methionine	UNP A0AAI7ZHB9
B	2	GLY	-	expression tag	UNP A0AAI7ZHB9
B	3	SER	-	expression tag	UNP A0AAI7ZHB9
B	4	SER	-	expression tag	UNP A0AAI7ZHB9
B	5	HIS	-	expression tag	UNP A0AAI7ZHB9
B	6	HIS	-	expression tag	UNP A0AAI7ZHB9
B	7	HIS	-	expression tag	UNP A0AAI7ZHB9
B	8	HIS	-	expression tag	UNP A0AAI7ZHB9
B	9	HIS	-	expression tag	UNP A0AAI7ZHB9
B	10	HIS	-	expression tag	UNP A0AAI7ZHB9
B	11	SER	-	expression tag	UNP A0AAI7ZHB9
B	12	SER	-	expression tag	UNP A0AAI7ZHB9
B	13	GLY	-	expression tag	UNP A0AAI7ZHB9
B	14	LEU	-	expression tag	UNP A0AAI7ZHB9
B	15	VAL	-	expression tag	UNP A0AAI7ZHB9
B	16	PRO	-	expression tag	UNP A0AAI7ZHB9
B	17	ARG	-	expression tag	UNP A0AAI7ZHB9
B	18	GLY	-	expression tag	UNP A0AAI7ZHB9
B	19	SER	-	expression tag	UNP A0AAI7ZHB9
C	1	MET	-	initiating methionine	UNP A0AAI7ZHB9
C	2	GLY	-	expression tag	UNP A0AAI7ZHB9
C	3	SER	-	expression tag	UNP A0AAI7ZHB9
C	4	SER	-	expression tag	UNP A0AAI7ZHB9
C	5	HIS	-	expression tag	UNP A0AAI7ZHB9
C	6	HIS	-	expression tag	UNP A0AAI7ZHB9
C	7	HIS	-	expression tag	UNP A0AAI7ZHB9
C	8	HIS	-	expression tag	UNP A0AAI7ZHB9
C	9	HIS	-	expression tag	UNP A0AAI7ZHB9
C	10	HIS	-	expression tag	UNP A0AAI7ZHB9
C	11	SER	-	expression tag	UNP A0AAI7ZHB9
C	12	SER	-	expression tag	UNP A0AAI7ZHB9
C	13	GLY	-	expression tag	UNP A0AAI7ZHB9
C	14	LEU	-	expression tag	UNP A0AAI7ZHB9
C	15	VAL	-	expression tag	UNP A0AAI7ZHB9
C	16	PRO	-	expression tag	UNP A0AAI7ZHB9
C	17	ARG	-	expression tag	UNP A0AAI7ZHB9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP A0AAI7ZHB9
C	19	SER	-	expression tag	UNP A0AAI7ZHB9
D	1	MET	-	initiating methionine	UNP A0AAI7ZHB9
D	2	GLY	-	expression tag	UNP A0AAI7ZHB9
D	3	SER	-	expression tag	UNP A0AAI7ZHB9
D	4	SER	-	expression tag	UNP A0AAI7ZHB9
D	5	HIS	-	expression tag	UNP A0AAI7ZHB9
D	6	HIS	-	expression tag	UNP A0AAI7ZHB9
D	7	HIS	-	expression tag	UNP A0AAI7ZHB9
D	8	HIS	-	expression tag	UNP A0AAI7ZHB9
D	9	HIS	-	expression tag	UNP A0AAI7ZHB9
D	10	HIS	-	expression tag	UNP A0AAI7ZHB9
D	11	SER	-	expression tag	UNP A0AAI7ZHB9
D	12	SER	-	expression tag	UNP A0AAI7ZHB9
D	13	GLY	-	expression tag	UNP A0AAI7ZHB9
D	14	LEU	-	expression tag	UNP A0AAI7ZHB9
D	15	VAL	-	expression tag	UNP A0AAI7ZHB9
D	16	PRO	-	expression tag	UNP A0AAI7ZHB9
D	17	ARG	-	expression tag	UNP A0AAI7ZHB9
D	18	GLY	-	expression tag	UNP A0AAI7ZHB9
D	19	SER	-	expression tag	UNP A0AAI7ZHB9
E	1	MET	-	initiating methionine	UNP A0AAI7ZHB9
E	2	GLY	-	expression tag	UNP A0AAI7ZHB9
E	3	SER	-	expression tag	UNP A0AAI7ZHB9
E	4	SER	-	expression tag	UNP A0AAI7ZHB9
E	5	HIS	-	expression tag	UNP A0AAI7ZHB9
E	6	HIS	-	expression tag	UNP A0AAI7ZHB9
E	7	HIS	-	expression tag	UNP A0AAI7ZHB9
E	8	HIS	-	expression tag	UNP A0AAI7ZHB9
E	9	HIS	-	expression tag	UNP A0AAI7ZHB9
E	10	HIS	-	expression tag	UNP A0AAI7ZHB9
E	11	SER	-	expression tag	UNP A0AAI7ZHB9
E	12	SER	-	expression tag	UNP A0AAI7ZHB9
E	13	GLY	-	expression tag	UNP A0AAI7ZHB9
E	14	LEU	-	expression tag	UNP A0AAI7ZHB9
E	15	VAL	-	expression tag	UNP A0AAI7ZHB9
E	16	PRO	-	expression tag	UNP A0AAI7ZHB9
E	17	ARG	-	expression tag	UNP A0AAI7ZHB9
E	18	GLY	-	expression tag	UNP A0AAI7ZHB9
E	19	SER	-	expression tag	UNP A0AAI7ZHB9
F	1	MET	-	initiating methionine	UNP A0AAI7ZHB9
F	2	GLY	-	expression tag	UNP A0AAI7ZHB9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	3	SER	-	expression tag	UNP A0AAI7ZHB9
F	4	SER	-	expression tag	UNP A0AAI7ZHB9
F	5	HIS	-	expression tag	UNP A0AAI7ZHB9
F	6	HIS	-	expression tag	UNP A0AAI7ZHB9
F	7	HIS	-	expression tag	UNP A0AAI7ZHB9
F	8	HIS	-	expression tag	UNP A0AAI7ZHB9
F	9	HIS	-	expression tag	UNP A0AAI7ZHB9
F	10	HIS	-	expression tag	UNP A0AAI7ZHB9
F	11	SER	-	expression tag	UNP A0AAI7ZHB9
F	12	SER	-	expression tag	UNP A0AAI7ZHB9
F	13	GLY	-	expression tag	UNP A0AAI7ZHB9
F	14	LEU	-	expression tag	UNP A0AAI7ZHB9
F	15	VAL	-	expression tag	UNP A0AAI7ZHB9
F	16	PRO	-	expression tag	UNP A0AAI7ZHB9
F	17	ARG	-	expression tag	UNP A0AAI7ZHB9
F	18	GLY	-	expression tag	UNP A0AAI7ZHB9
F	19	SER	-	expression tag	UNP A0AAI7ZHB9
G	1	MET	-	initiating methionine	UNP A0AAI7ZHB9
G	2	GLY	-	expression tag	UNP A0AAI7ZHB9
G	3	SER	-	expression tag	UNP A0AAI7ZHB9
G	4	SER	-	expression tag	UNP A0AAI7ZHB9
G	5	HIS	-	expression tag	UNP A0AAI7ZHB9
G	6	HIS	-	expression tag	UNP A0AAI7ZHB9
G	7	HIS	-	expression tag	UNP A0AAI7ZHB9
G	8	HIS	-	expression tag	UNP A0AAI7ZHB9
G	9	HIS	-	expression tag	UNP A0AAI7ZHB9
G	10	HIS	-	expression tag	UNP A0AAI7ZHB9
G	11	SER	-	expression tag	UNP A0AAI7ZHB9
G	12	SER	-	expression tag	UNP A0AAI7ZHB9
G	13	GLY	-	expression tag	UNP A0AAI7ZHB9
G	14	LEU	-	expression tag	UNP A0AAI7ZHB9
G	15	VAL	-	expression tag	UNP A0AAI7ZHB9
G	16	PRO	-	expression tag	UNP A0AAI7ZHB9
G	17	ARG	-	expression tag	UNP A0AAI7ZHB9
G	18	GLY	-	expression tag	UNP A0AAI7ZHB9
G	19	SER	-	expression tag	UNP A0AAI7ZHB9
H	1	MET	-	initiating methionine	UNP A0AAI7ZHB9
H	2	GLY	-	expression tag	UNP A0AAI7ZHB9
H	3	SER	-	expression tag	UNP A0AAI7ZHB9
H	4	SER	-	expression tag	UNP A0AAI7ZHB9
H	5	HIS	-	expression tag	UNP A0AAI7ZHB9
H	6	HIS	-	expression tag	UNP A0AAI7ZHB9

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Chain	Residue	Modelled	Actual	Comment	Reference
H	7	HIS	-	expression tag	UNP A0AAI7ZHB9
H	8	HIS	-	expression tag	UNP A0AAI7ZHB9
H	9	HIS	-	expression tag	UNP A0AAI7ZHB9
H	10	HIS	-	expression tag	UNP A0AAI7ZHB9
H	11	SER	-	expression tag	UNP A0AAI7ZHB9
H	12	SER	-	expression tag	UNP A0AAI7ZHB9
H	13	GLY	-	expression tag	UNP A0AAI7ZHB9
H	14	LEU	-	expression tag	UNP A0AAI7ZHB9
H	15	VAL	-	expression tag	UNP A0AAI7ZHB9
H	16	PRO	-	expression tag	UNP A0AAI7ZHB9
H	17	ARG	-	expression tag	UNP A0AAI7ZHB9
H	18	GLY	-	expression tag	UNP A0AAI7ZHB9
H	19	SER	-	expression tag	UNP A0AAI7ZHB9

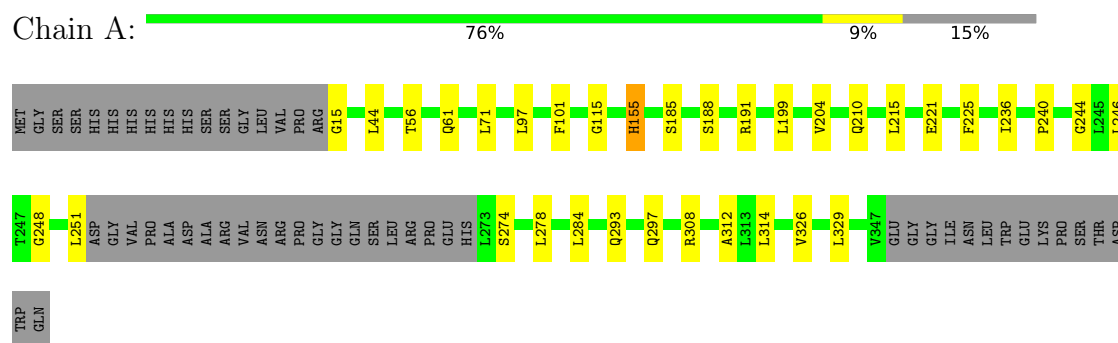
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	E	1	Total O 1 1	0	0

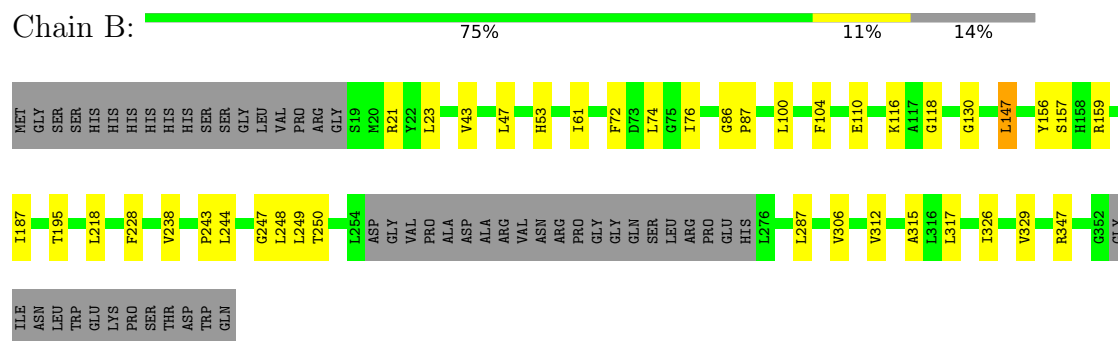
3 Residue-property plots [i](#)

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.

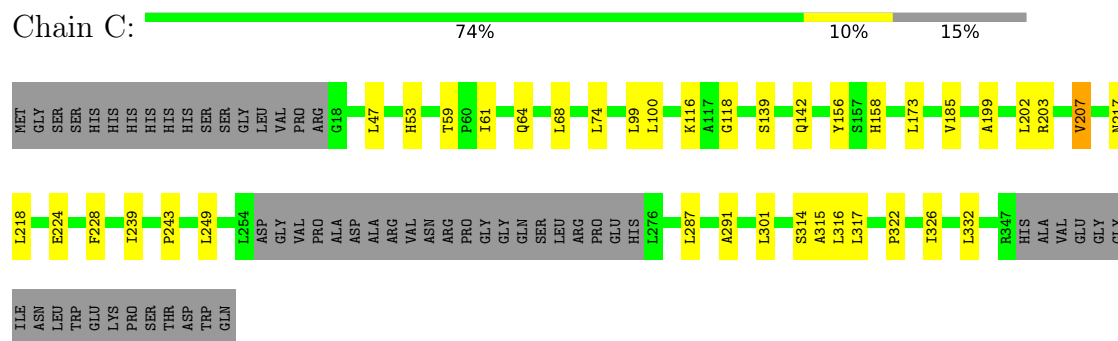
• Molecule 1: Oxidoreductase



• Molecule 1: Oxidoreductase

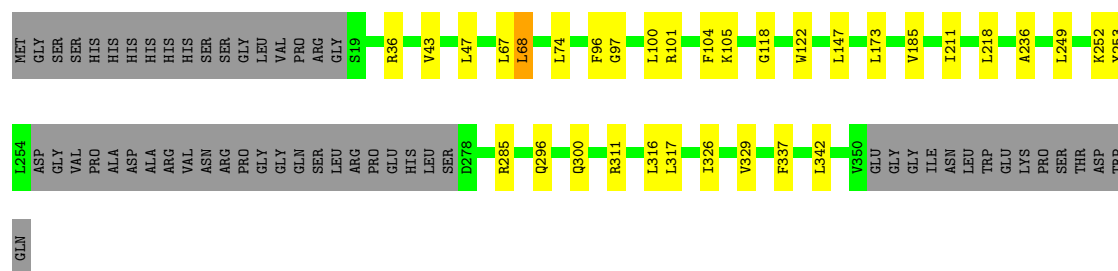


• Molecule 1: Oxidoreductase



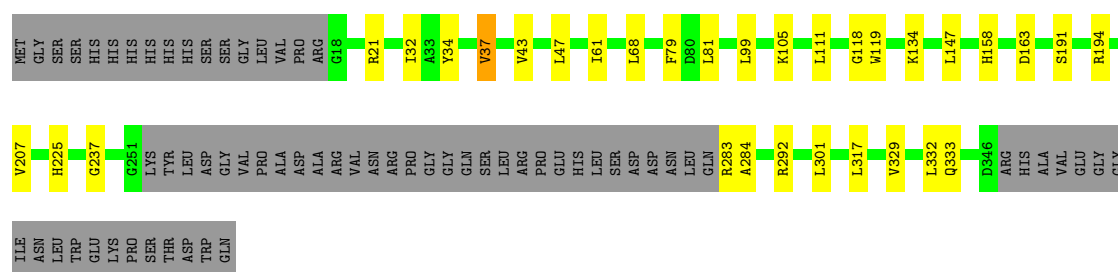
• Molecule 1: Oxidoreductase

Chain D:  76% 9% 15%



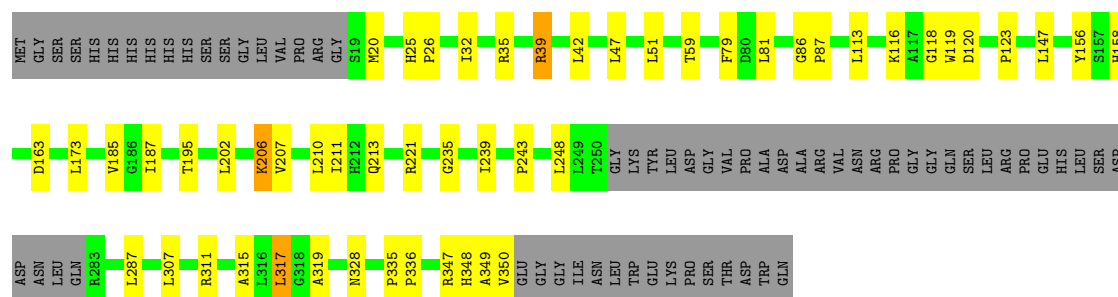
• Molecule 1: Oxidoreductase

Chain E:  73% 8% 18%



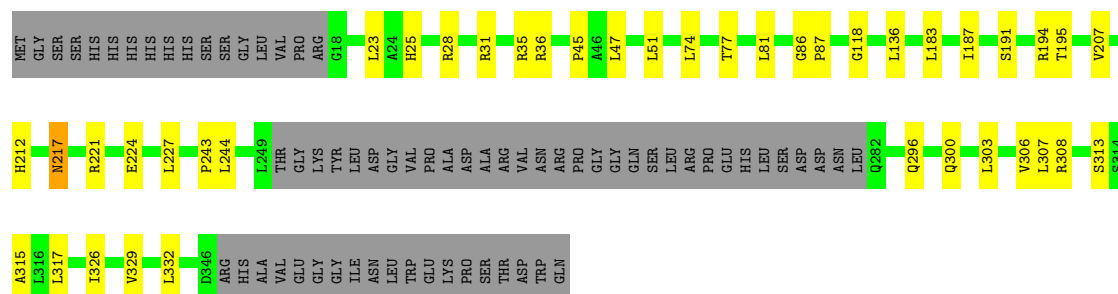
• Molecule 1: Oxidoreductase

Chain F:  68% 13% 18%



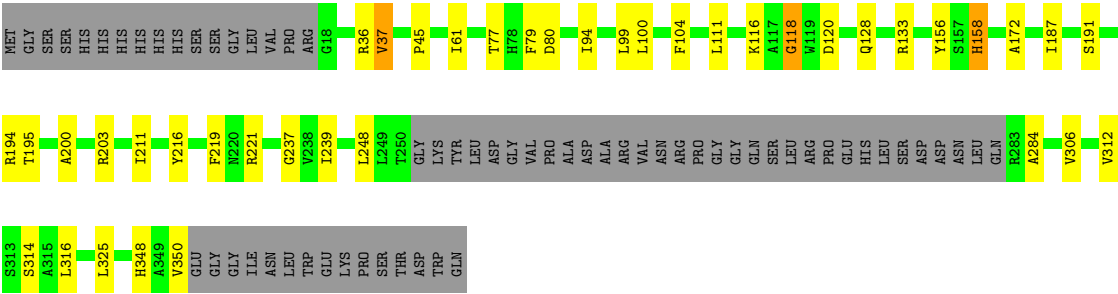
• Molecule 1: Oxidoreductase

Chain G:  70% 11% 19%



• Molecule 1: Oxidoreductase

Chain H: 71% 10% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	129.62Å 129.76Å 228.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.84 – 2.98 85.84 – 2.98	Depositor EDS
% Data completeness (in resolution range)	69.2 (85.84-2.98) 59.9 (85.84-2.98)	Depositor EDS
R_{merge}	0.54	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.231 , 0.276 0.233 , 0.278	Depositor DCC
R_{free} test set	5468 reflections (6.86%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.195 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19052	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6743e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.08	0/2494	0.23	0/3388
1	B	0.07	0/2503	0.23	0/3400
1	C	0.07	0/2471	0.22	0/3356
1	D	0.08	0/2476	0.21	0/3364
1	E	0.07	0/2375	0.23	0/3227
1	F	0.07	0/2401	0.24	0/3263
1	G	0.08	0/2373	0.23	0/3224
1	H	0.07	0/2405	0.22	0/3268
All	All	0.07	0/19498	0.23	0/26490

There are no bond length outliers.

There are no bond angle outliers.

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	2437	0	2403	19	0
1	B	2446	0	2409	21	0
1	C	2415	0	2382	20	0
1	D	2419	0	2384	19	0
1	E	2320	0	2287	16	0
1	F	2345	0	2315	24	0
1	G	2318	0	2285	21	0
1	H	2349	0	2318	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
All	All	19052	0	18783	152	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 4.

All (152) 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:G:306:VAL:HG23	1:G:307:LEU:HD12	1.71	0.72
1:F:39:ARG:HE	1:F:235:GLY:HA2	1.58	0.69
1:F:116:LYS:HG2	1:F:156:TYR:HB2	1.78	0.66
1:A:215:LEU:HD13	1:A:284:LEU:HD13	1.78	0.64
1:F:51:LEU:HD13	1:F:81:LEU:HG	1.78	0.64
1:H:239:ILE:HG12	1:H:314:SER:HB2	1.78	0.64
1:A:56:THR:HB	1:A:61:GLN:HE21	1.63	0.63
1:H:116:LYS:HG2	1:H:156:TYR:HB2	1.81	0.63
1:H:191:SER:HB3	1:H:194:ARG:HD2	1.82	0.62
1:E:191:SER:HB2	1:E:194:ARG:HB2	1.83	0.61
1:A:71:LEU:HD13	1:A:326:VAL:HG21	1.81	0.61
1:A:274:SER:HA	1:A:278:LEU:HD23	1.81	0.61
1:D:74:LEU:HD11	1:D:326:ILE:HG12	1.82	0.60
1:D:252:LYS:HE3	1:D:253:TYR:HE1	1.65	0.60
1:D:47:LEU:HD12	1:D:329:VAL:HA	1.83	0.60
1:C:116:LYS:HG2	1:C:156:TYR:HB2	1.84	0.59
1:G:191:SER:HB2	1:G:194:ARG:HG2	1.83	0.59
1:D:47:LEU:HD13	1:D:317:LEU:HD11	1.83	0.59
1:C:218:LEU:HD13	1:C:287:LEU:HD13	1.83	0.59
1:B:244:LEU:HD13	1:B:250:THR:HG22	1.86	0.58
1:B:187:ILE:HD11	1:B:195:THR:HG23	1.84	0.58
1:A:225:PHE:HB3	1:A:308:ARG:HD2	1.86	0.58
1:A:44:LEU:HD12	1:A:326:VAL:HA	1.86	0.57
1:H:219:PHE:HZ	1:H:284:ALA:HB2	1.69	0.57
1:A:188:SER:HB3	1:A:191:ARG:HB2	1.87	0.57
1:A:240:PRO:HG3	1:A:312:ALA:HB1	1.87	0.56
1:C:217:ASN:HB3	1:C:243:PRO:HA	1.86	0.56
1:G:74:LEU:HD21	1:G:326:ILE:HG22	1.86	0.56
1:C:74:LEU:HD11	1:C:326:ILE:HD13	1.86	0.56
1:F:35:ARG:HH12	1:F:307:LEU:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:211:ILE:HD11	1:H:239:ILE:HG13	1.87	0.56
1:D:100:LEU:HD12	1:D:104:PHE:HB2	1.86	0.56
1:E:81:LEU:HD22	1:E:147:LEU:HD21	1.88	0.55
1:A:15:GLY:HA3	1:F:123:PRO:HG3	1.88	0.55
1:F:51:LEU:HD11	1:F:79:PHE:HB3	1.87	0.55
1:B:157:SER:HB3	1:B:187:ILE:HG22	1.90	0.54
1:F:243:PRO:HG3	1:F:315:ALA:HB1	1.88	0.54
1:F:173:LEU:HB3	1:F:185:VAL:HG11	1.90	0.53
1:F:317:LEU:HD11	1:F:328:ASN:HB3	1.90	0.53
1:C:239:ILE:HG13	1:C:314:SER:HB2	1.91	0.53
1:C:243:PRO:HG3	1:C:315:ALA:HB1	1.92	0.52
1:H:120:ASP:HA	1:H:128:GLN:HA	1.91	0.52
1:H:306:VAL:HG12	1:H:312:VAL:HG11	1.91	0.52
1:B:47:LEU:HD12	1:B:329:VAL:HA	1.91	0.52
1:F:287:LEU:HD11	1:F:349:ALA:HB2	1.91	0.52
1:E:32:ILE:HD11	1:E:329:VAL:HG22	1.91	0.52
1:H:221:ARG:HD3	1:H:350:VAL:H	1.75	0.52
1:C:332:LEU:HD23	1:C:332:LEU:H	1.75	0.52
1:A:155:HIS:HA	1:A:185:SER:HB3	1.93	0.51
1:C:291:ALA:HB2	1:C:301:LEU:HD22	1.91	0.51
1:E:37:VAL:HG23	1:E:237:GLY:HA3	1.90	0.51
1:H:200:ALA:HA	1:H:203:ARG:HE	1.74	0.51
1:H:37:VAL:HG23	1:H:237:GLY:HA3	1.91	0.51
1:A:44:LEU:HD13	1:A:314:LEU:HD11	1.91	0.51
1:G:187:ILE:HD11	1:G:195:THR:HG23	1.93	0.50
1:E:317:LEU:H	1:E:317:LEU:HD23	1.76	0.50
1:G:28:ARG:HA	1:G:31:ARG:HD3	1.93	0.50
1:B:74:LEU:HD11	1:B:326:ILE:HG12	1.93	0.50
1:D:218:LEU:HB2	1:D:249:LEU:HD11	1.94	0.50
1:E:163:ASP:HB3	1:G:36:ARG:HH21	1.76	0.50
1:A:293:GLN:HB3	1:A:297:GLN:HB2	1.93	0.50
1:H:100:LEU:HD12	1:H:104:PHE:HB2	1.94	0.49
1:G:35:ARG:HD2	1:G:313:SER:HA	1.94	0.49
1:F:317:LEU:HD22	1:F:319:ALA:HB2	1.94	0.49
1:H:118:GLY:HA3	1:H:158:HIS:HB3	1.95	0.49
1:D:74:LEU:HD13	1:D:329:VAL:HG21	1.95	0.49
1:G:243:PRO:HG3	1:G:315:ALA:HB1	1.94	0.48
1:F:51:LEU:HD22	1:F:81:LEU:HD21	1.95	0.48
1:G:74:LEU:HD13	1:G:329:VAL:HG21	1.95	0.48
1:A:329:LEU:H	1:A:329:LEU:HD23	1.79	0.48
1:D:211:ILE:HA	1:D:236:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:PHE:HB3	1:D:342:LEU:HG	1.96	0.47
1:H:133:ARG:HG3	1:H:172:ALA:HB2	1.96	0.47
1:F:32:ILE:HD11	1:F:47:LEU:H	1.80	0.47
1:C:59:THR:HB	1:C:64:GLN:HE21	1.80	0.47
1:E:47:LEU:HD12	1:E:317:LEU:HD22	1.97	0.47
1:B:47:LEU:HD13	1:B:317:LEU:HD11	1.96	0.46
1:B:116:LYS:HG2	1:B:156:TYR:HB2	1.96	0.46
1:E:79:PHE:HE2	1:E:111:LEU:HD22	1.79	0.46
1:G:45:PRO:HG3	1:G:77:THR:H	1.81	0.46
1:B:218:LEU:HD13	1:B:287:LEU:HD13	1.98	0.46
1:C:224:GLU:HA	1:C:228:PHE:HD2	1.80	0.46
1:E:68:LEU:HD12	1:E:99:LEU:HD23	1.97	0.46
1:B:306:VAL:HG12	1:B:312:VAL:HG11	1.98	0.46
1:C:47:LEU:HD22	1:C:317:LEU:HD11	1.98	0.46
1:C:218:LEU:HD12	1:C:249:LEU:HD13	1.97	0.46
1:G:47:LEU:HD22	1:G:317:LEU:HD11	1.97	0.45
1:B:86:GLY:HA3	1:B:87:PRO:HA	1.88	0.45
1:G:296:GLN:HB3	1:G:300:GLN:HB2	1.98	0.45
1:B:61:ILE:HG13	1:E:61:ILE:HD11	1.97	0.45
1:F:187:ILE:HD11	1:F:195:THR:HG23	1.98	0.45
1:G:221:ARG:HH21	1:G:308:ARG:HH22	1.64	0.45
1:C:199:ALA:O	1:C:203:ARG:HG2	2.16	0.45
1:G:217:ASN:HD22	1:G:217:ASN:HA	1.68	0.45
1:C:116:LYS:HD3	1:C:158:HIS:CD2	2.52	0.45
1:A:97:LEU:HA	1:A:101:PHE:HB2	1.99	0.44
1:A:221:GLU:HA	1:A:225:PHE:HD2	1.83	0.44
1:B:147:LEU:HD13	1:B:147:LEU:HA	1.88	0.44
1:F:211:ILE:HD11	1:F:239:ILE:HB	1.98	0.44
1:B:21:ARG:HD3	1:B:21:ARG:HA	1.70	0.44
1:F:42:LEU:HD23	1:F:210:LEU:HD21	2.00	0.44
1:D:173:LEU:HB3	1:D:185:VAL:HG11	2.00	0.43
1:F:86:GLY:HA3	1:F:87:PRO:HA	1.89	0.43
1:G:51:LEU:HD13	1:G:81:LEU:HG	1.99	0.43
1:B:130:GLY:H	1:B:159:ARG:HH21	1.66	0.43
1:B:228:PHE:HE1	1:B:238:VAL:HG11	1.83	0.43
1:B:110:GLU:HG2	1:D:122:TRP:CD1	2.53	0.43
1:D:101:ARG:HA	1:D:105:LYS:HD3	2.01	0.43
1:D:316:LEU:HD23	1:D:316:LEU:HA	1.93	0.43
1:A:244:GLY:C	1:A:246:LEU:H	2.27	0.42
1:B:100:LEU:HA	1:B:104:PHE:HB2	2.01	0.42
1:E:134:LYS:HA	1:G:183:LEU:HD13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:PRO:HG2	1:H:77:THR:H	1.85	0.42
1:A:248:GLY:HA2	1:A:251:LEU:HD13	2.00	0.42
1:C:61:ILE:HD11	1:H:61:ILE:HD11	2.01	0.42
1:F:81:LEU:HD13	1:F:147:LEU:HD21	2.00	0.42
1:G:212:HIS:CE1	1:G:227:LEU:HD21	2.54	0.42
1:D:97:GLY:O	1:D:101:ARG:HG3	2.20	0.42
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.92	0.42
1:E:119:TRP:HD1	1:E:158:HIS:CG	2.37	0.42
1:F:163:ASP:HB3	1:H:36:ARG:CZ	2.48	0.42
1:B:72:PHE:H	1:B:76:ILE:HB	1.85	0.42
1:C:322:PRO:O	1:C:326:ILE:HG12	2.19	0.42
1:F:206:LYS:HE2	1:F:206:LYS:HB2	1.94	0.42
1:A:210:GLN:HG3	1:A:236:ILE:HG23	2.02	0.42
1:D:296:GLN:HB3	1:D:300:GLN:HB2	2.02	0.42
1:D:68:LEU:HD21	1:D:96:PHE:CD1	2.55	0.42
1:E:34:TYR:HB3	1:E:43:VAL:HG12	2.01	0.42
1:E:283:ARG:HB3	1:E:284:ALA:H	1.57	0.42
1:F:119:TRP:HB3	1:F:120:ASP:H	1.69	0.41
1:H:187:ILE:HD11	1:H:195:THR:HG23	2.03	0.41
1:F:335:PRO:HA	1:F:336:PRO:HD3	1.95	0.41
1:E:105:LYS:HD2	1:E:105:LYS:HA	1.81	0.41
1:H:80:ASP:HB3	1:H:316:LEU:HD21	2.03	0.41
1:B:23:LEU:HD22	1:G:23:LEU:HD22	2.03	0.41
1:C:139:SER:HA	1:C:142:GLN:HG2	2.01	0.41
1:C:202:LEU:HB3	1:C:207:VAL:O	2.21	0.41
1:F:25:HIS:ND1	1:F:26:PRO:HD2	2.36	0.41
1:G:244:LEU:HD21	1:G:303:LEU:HG	2.02	0.41
1:B:243:PRO:HG3	1:B:315:ALA:HB1	2.01	0.41
1:D:36:ARG:HA	1:D:43:VAL:HG12	2.02	0.41
1:G:86:GLY:HA3	1:G:87:PRO:HA	1.92	0.41
1:C:173:LEU:HB3	1:C:185:VAL:HG11	2.03	0.41
1:D:311:ARG:HE	1:D:311:ARG:HB2	1.70	0.41
1:A:199:LEU:HB3	1:A:204:VAL:O	2.21	0.40
1:C:68:LEU:HD12	1:C:99:LEU:HG	2.03	0.40
1:E:292:ARG:HA	1:E:292:ARG:HD3	1.89	0.40
1:F:213:GLN:HG3	1:F:239:ILE:HG23	2.03	0.40
1:H:79:PHE:HE2	1:H:111:LEU:HD22	1.86	0.40
1:G:136:LEU:HD23	1:G:136:LEU:HA	1.96	0.40
1:H:216:TYR:HD2	1:H:306:VAL:HG13	1.86	0.40
1:B:247:GLY:O	1:B:248:LEU:HB2	2.21	0.40

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	308/365 (84%)	291 (94%)	16 (5%)	1 (0%)	36	67
1	B	309/365 (85%)	288 (93%)	20 (6%)	1 (0%)	36	67
1	C	305/365 (84%)	291 (95%)	13 (4%)	1 (0%)	36	67
1	D	305/365 (84%)	292 (96%)	12 (4%)	1 (0%)	36	67
1	E	294/365 (80%)	277 (94%)	15 (5%)	2 (1%)	18	50
1	F	296/365 (81%)	281 (95%)	14 (5%)	1 (0%)	36	67
1	G	293/365 (80%)	267 (91%)	25 (8%)	1 (0%)	36	67
1	H	297/365 (81%)	270 (91%)	26 (9%)	1 (0%)	36	67
All	All	2407/2920 (82%)	2257 (94%)	141 (6%)	9 (0%)	30	62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	118	GLY
1	D	118	GLY
1	E	225	HIS
1	G	118	GLY
1	A	115	GLY
1	H	118	GLY
1	B	118	GLY
1	E	118	GLY
1	F	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	245/289 (85%)	244 (100%)	1 (0%)	84	90
1	B	246/289 (85%)	241 (98%)	5 (2%)	48	75
1	C	243/289 (84%)	239 (98%)	4 (2%)	55	78
1	D	243/289 (84%)	239 (98%)	4 (2%)	55	78
1	E	232/289 (80%)	226 (97%)	6 (3%)	40	70
1	F	235/289 (81%)	220 (94%)	15 (6%)	16	45
1	G	232/289 (80%)	227 (98%)	5 (2%)	45	73
1	H	235/289 (81%)	228 (97%)	7 (3%)	36	67
All	All	1911/2312 (83%)	1864 (98%)	47 (2%)	42	71

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	B	43	VAL
1	B	53	HIS
1	B	147	LEU
1	B	249	LEU
1	B	347	ARG
1	C	53	HIS
1	C	100	LEU
1	C	207	VAL
1	C	316	LEU
1	D	67	LEU
1	D	68	LEU
1	D	147	LEU
1	D	285	ARG
1	E	21	ARG
1	E	37	VAL
1	E	207	VAL
1	E	301	LEU
1	E	332	LEU
1	E	333	GLN
1	F	20	MET
1	F	39	ARG
1	F	59	THR
1	F	113	LEU
1	F	158	HIS

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Mol	Chain	Res	Type
1	F	202	LEU
1	F	206	LYS
1	F	207	VAL
1	F	221	ARG
1	F	248	LEU
1	F	311	ARG
1	F	317	LEU
1	F	347	ARG
1	F	348	HIS
1	F	350	VAL
1	G	25	HIS
1	G	207	VAL
1	G	217	ASN
1	G	224	GLU
1	G	332	LEU
1	H	37	VAL
1	H	94	ILE
1	H	99	LEU
1	H	158	HIS
1	H	248	LEU
1	H	325	LEU
1	H	348	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	176	GLN
1	B	324	GLN
1	C	64	GLN
1	C	95	ASN
1	C	282	GLN
1	D	142	GLN
1	D	220	ASN
1	F	54	ASN
1	F	179	GLN
1	F	212	HIS
1	G	212	HIS
1	G	213	GLN
1	G	328	ASN
1	G	333	GLN
1	H	54	ASN

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Mol	Chain	Res	Type
1	H	128	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	312/365 (85%)	-1.55	0 100 100	15, 33, 66, 89	0
1	B	313/365 (85%)	-1.57	0 100 100	12, 32, 61, 86	0
1	C	309/365 (84%)	-1.56	0 100 100	12, 32, 63, 87	0
1	D	309/365 (84%)	-1.61	0 100 100	13, 33, 59, 82	0
1	E	298/365 (81%)	-1.33	0 100 100	22, 49, 91, 111	0
1	F	300/365 (82%)	-1.38	0 100 100	22, 51, 85, 113	0
1	G	297/365 (81%)	-1.44	0 100 100	23, 48, 76, 90	0
1	H	301/365 (82%)	-1.40	0 100 100	21, 50, 88, 106	0
All	All	2439/2920 (83%)	-1.48	0 100 100	12, 40, 80, 113	0

There are no RSRZ outliers to report.

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.