



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 07:50 AM EDT

PDB ID : 3A17
Title : Crystal Structure of Aldoxime Dehydratase (OxdRE) in Complex with Butyraldoxime (Co-crystal)
Authors : Sawai, H.; Sugimoto, H.; Kato, Y.; Asano, Y.; Shiro, Y.; Aono, S.
Deposited on : unknown
Resolution : 2.50 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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

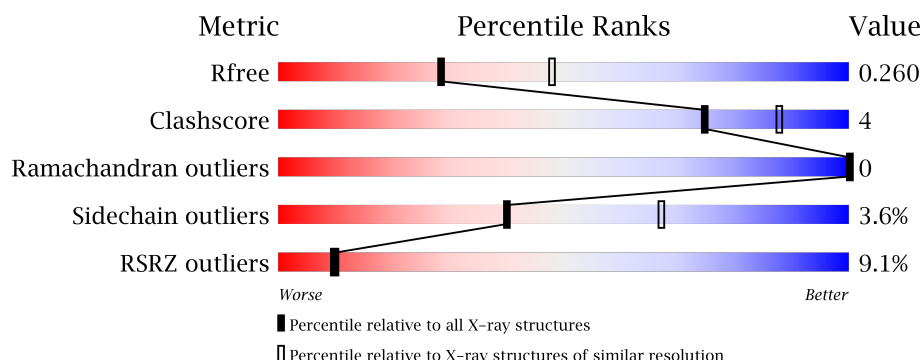
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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 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	373	<div> <div>5%</div> <div>83% 10% 6%</div> </div>
1	B	373	<div> <div>11%</div> <div>87% 8% . .</div> </div>
1	C	373	<div> <div>6%</div> <div>84% 10% . 6%</div> </div>
1	D	373	<div> <div>10%</div> <div>85% 10% . .</div> </div>
1	E	373	<div> <div>7%</div> <div>87% 7% 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	373	<div><div></div><div>12%</div><div>86%</div><div>10%</div><div></div><div></div></div>
1	G	373	<div><div></div><div>6%</div><div>85%</div><div>9%</div><div></div><div>5%</div></div>
1	H	373	<div><div></div><div>13%</div><div>85%</div><div>11%</div><div></div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23656 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 Aldoxime dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2790	1757	492	529	12			
1	B	359	Total	C	N	O	S	0	0	0
			2853	1795	506	540	12			
1	C	352	Total	C	N	O	S	0	1	0
			2812	1770	497	533	12			
1	D	360	Total	C	N	O	S	0	1	0
			2866	1803	510	541	12			
1	E	351	Total	C	N	O	S	0	1	0
			2803	1765	496	530	12			
1	F	359	Total	C	N	O	S	0	0	0
			2853	1795	506	540	12			
1	G	353	Total	C	N	O	S	0	0	0
			2815	1771	497	535	12			
1	H	359	Total	C	N	O	S	0	0	0
			2853	1795	506	540	12			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
A	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
A	-17	SER	-	EXPRESSION TAG	UNP Q76K71
A	-16	SER	-	EXPRESSION TAG	UNP Q76K71
A	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
A	-9	SER	-	EXPRESSION TAG	UNP Q76K71
A	-8	SER	-	EXPRESSION TAG	UNP Q76K71
A	-7	GLY	-	EXPRESSION TAG	UNP Q76K71

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
A	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
A	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
A	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
A	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
A	-1	SER	-	EXPRESSION TAG	UNP Q76K71
A	0	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
B	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
B	-17	SER	-	EXPRESSION TAG	UNP Q76K71
B	-16	SER	-	EXPRESSION TAG	UNP Q76K71
B	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
B	-9	SER	-	EXPRESSION TAG	UNP Q76K71
B	-8	SER	-	EXPRESSION TAG	UNP Q76K71
B	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
B	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
B	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
B	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
B	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
B	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
B	-1	SER	-	EXPRESSION TAG	UNP Q76K71
B	0	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
C	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
C	-17	SER	-	EXPRESSION TAG	UNP Q76K71
C	-16	SER	-	EXPRESSION TAG	UNP Q76K71
C	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
C	-9	SER	-	EXPRESSION TAG	UNP Q76K71
C	-8	SER	-	EXPRESSION TAG	UNP Q76K71
C	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
C	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
C	-5	VAL	-	EXPRESSION TAG	UNP Q76K71

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
C	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
C	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
C	-1	SER	-	EXPRESSION TAG	UNP Q76K71
C	0	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
D	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
D	-17	SER	-	EXPRESSION TAG	UNP Q76K71
D	-16	SER	-	EXPRESSION TAG	UNP Q76K71
D	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
D	-9	SER	-	EXPRESSION TAG	UNP Q76K71
D	-8	SER	-	EXPRESSION TAG	UNP Q76K71
D	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
D	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
D	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
D	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
D	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
D	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
D	-1	SER	-	EXPRESSION TAG	UNP Q76K71
D	0	HIS	-	EXPRESSION TAG	UNP Q76K71
E	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
E	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
E	-17	SER	-	EXPRESSION TAG	UNP Q76K71
E	-16	SER	-	EXPRESSION TAG	UNP Q76K71
E	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
E	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
E	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
E	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
E	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
E	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
E	-9	SER	-	EXPRESSION TAG	UNP Q76K71
E	-8	SER	-	EXPRESSION TAG	UNP Q76K71
E	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
E	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
E	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
E	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
E	-3	ARG	-	EXPRESSION TAG	UNP Q76K71

Continued on next page...

Continued from previous page...

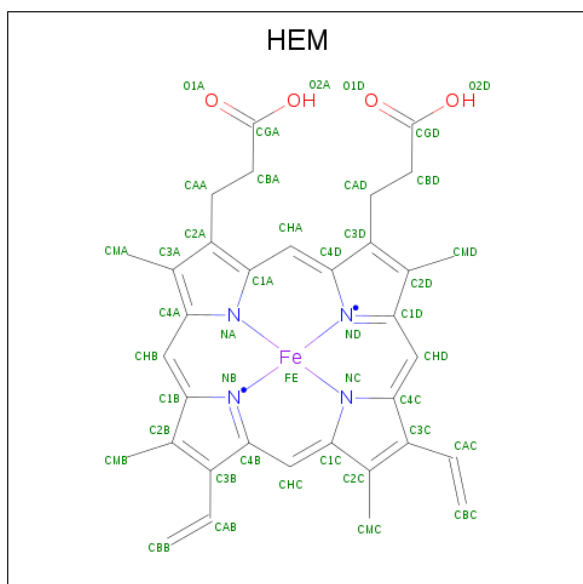
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
E	-1	SER	-	EXPRESSION TAG	UNP Q76K71
E	0	HIS	-	EXPRESSION TAG	UNP Q76K71
F	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
F	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
F	-17	SER	-	EXPRESSION TAG	UNP Q76K71
F	-16	SER	-	EXPRESSION TAG	UNP Q76K71
F	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
F	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
F	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
F	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
F	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
F	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
F	-9	SER	-	EXPRESSION TAG	UNP Q76K71
F	-8	SER	-	EXPRESSION TAG	UNP Q76K71
F	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
F	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
F	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
F	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
F	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
F	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
F	-1	SER	-	EXPRESSION TAG	UNP Q76K71
F	0	HIS	-	EXPRESSION TAG	UNP Q76K71
G	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
G	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
G	-17	SER	-	EXPRESSION TAG	UNP Q76K71
G	-16	SER	-	EXPRESSION TAG	UNP Q76K71
G	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
G	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
G	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
G	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
G	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
G	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
G	-9	SER	-	EXPRESSION TAG	UNP Q76K71
G	-8	SER	-	EXPRESSION TAG	UNP Q76K71
G	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
G	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
G	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
G	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
G	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
G	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
G	-1	SER	-	EXPRESSION TAG	UNP Q76K71

Continued on next page...

Continued from previous page...

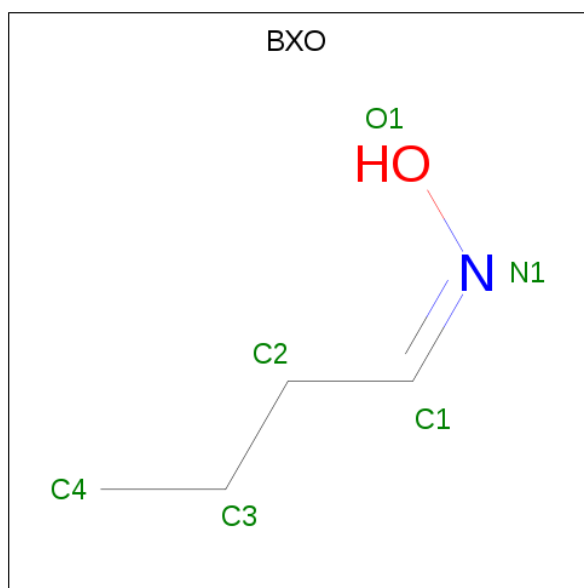
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	EXPRESSION TAG	UNP Q76K71
H	-19	MET	-	INITIATING METHIONINE	UNP Q76K71
H	-18	GLY	-	EXPRESSION TAG	UNP Q76K71
H	-17	SER	-	EXPRESSION TAG	UNP Q76K71
H	-16	SER	-	EXPRESSION TAG	UNP Q76K71
H	-15	HIS	-	EXPRESSION TAG	UNP Q76K71
H	-14	HIS	-	EXPRESSION TAG	UNP Q76K71
H	-13	HIS	-	EXPRESSION TAG	UNP Q76K71
H	-12	HIS	-	EXPRESSION TAG	UNP Q76K71
H	-11	HIS	-	EXPRESSION TAG	UNP Q76K71
H	-10	HIS	-	EXPRESSION TAG	UNP Q76K71
H	-9	SER	-	EXPRESSION TAG	UNP Q76K71
H	-8	SER	-	EXPRESSION TAG	UNP Q76K71
H	-7	GLY	-	EXPRESSION TAG	UNP Q76K71
H	-6	LEU	-	EXPRESSION TAG	UNP Q76K71
H	-5	VAL	-	EXPRESSION TAG	UNP Q76K71
H	-4	PRO	-	EXPRESSION TAG	UNP Q76K71
H	-3	ARG	-	EXPRESSION TAG	UNP Q76K71
H	-2	GLY	-	EXPRESSION TAG	UNP Q76K71
H	-1	SER	-	EXPRESSION TAG	UNP Q76K71
H	0	HIS	-	EXPRESSION TAG	UNP Q76K71

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (1Z)-butanal oxime (three-letter code: BXO) (formula: C₄H₉NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	4	1	1		
3	B	1	Total	C	N	O	0	0
			6	4	1	1		
3	C	1	Total	C	N	O	0	0
			6	4	1	1		
3	D	1	Total	C	N	O	0	0
			6	4	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			6	4	1	1		
3	F	1	Total	C	N	O	0	0
			6	4	1	1		
3	G	1	Total	C	N	O	0	0
			6	4	1	1		
3	H	1	Total	C	N	O	0	0
			6	4	1	1		

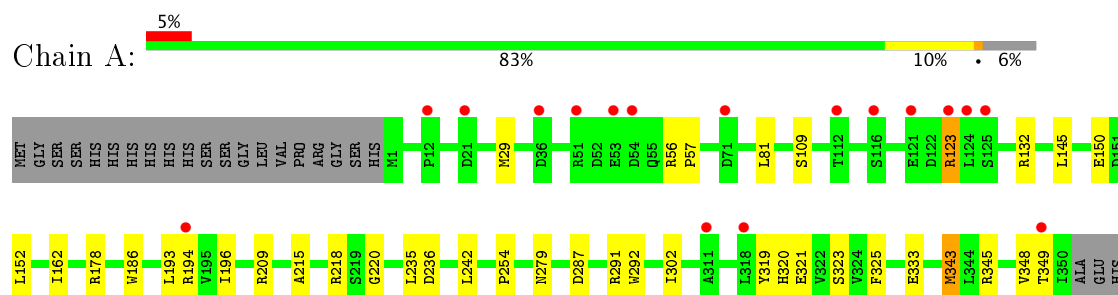
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	60	Total	O	0	0
			60	60		
4	C	93	Total	O	0	0
			93	93		
4	D	77	Total	O	0	0
			77	77		
4	E	83	Total	O	0	0
			83	83		
4	F	58	Total	O	0	0
			58	58		
4	G	84	Total	O	0	0
			84	84		
4	H	59	Total	O	0	0
			59	59		

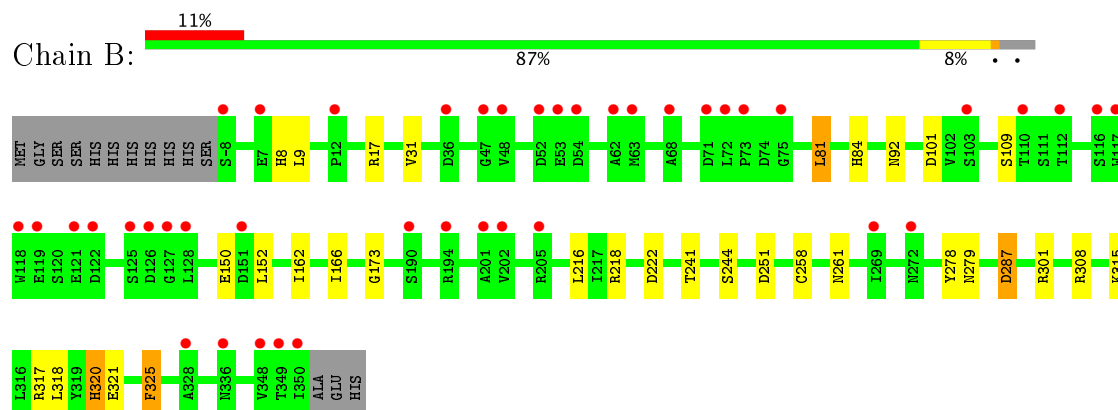
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

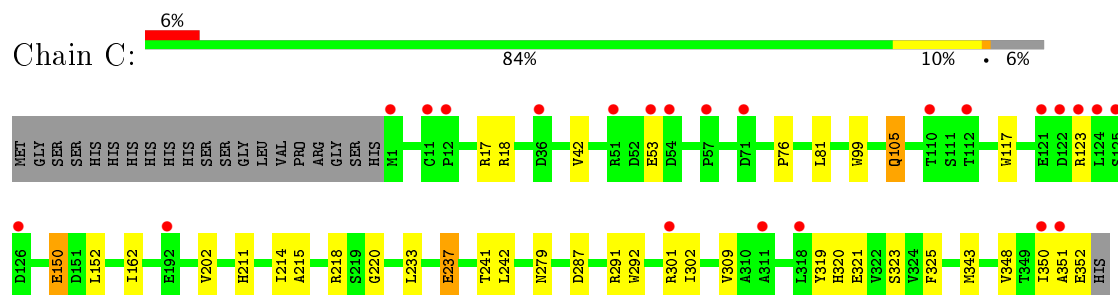
• Molecule 1: Aldoxime dehydratase



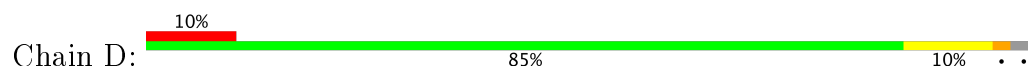
• Molecule 1: Aldoxime dehydratase

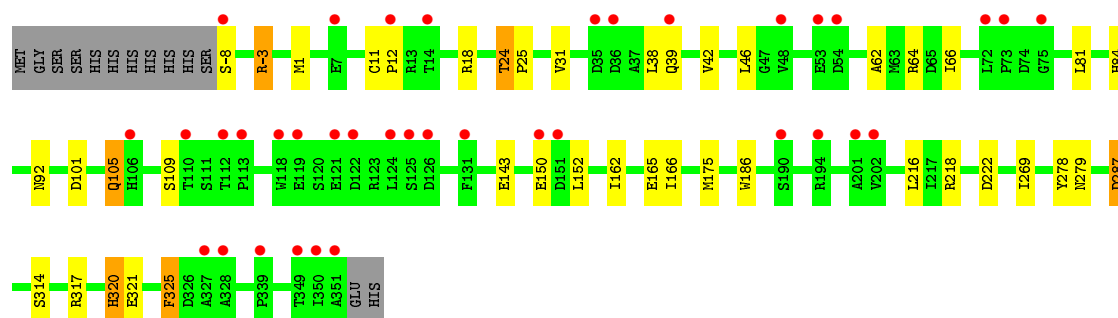


• Molecule 1: Aldoxime dehydratase

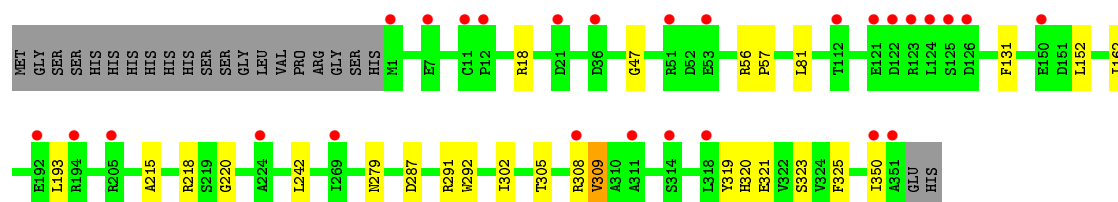
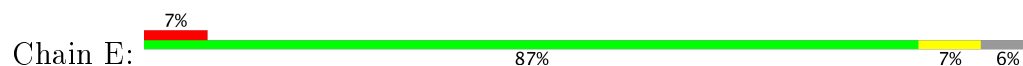


• Molecule 1: Aldoxime dehydratase

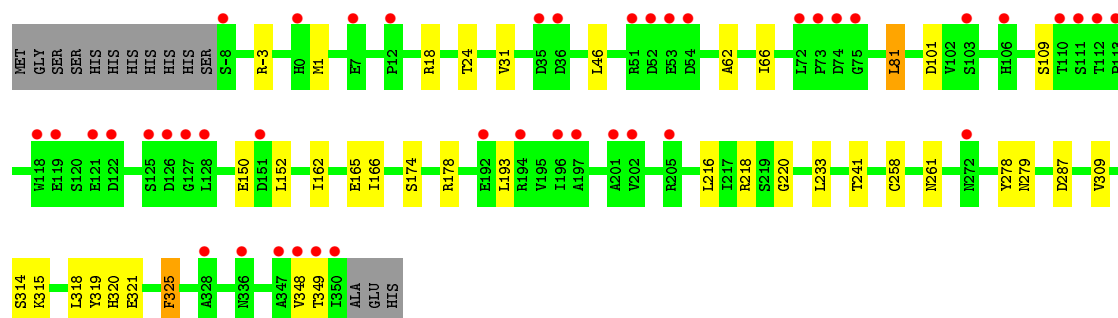
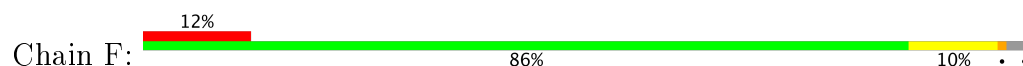




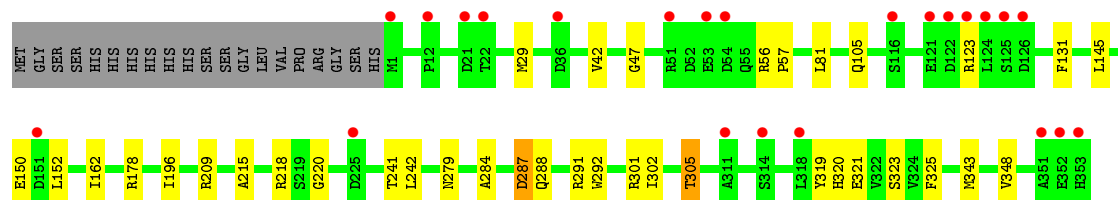
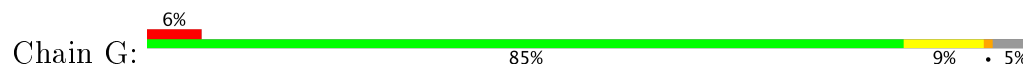
- Molecule 1: Aldoxime dehydratase



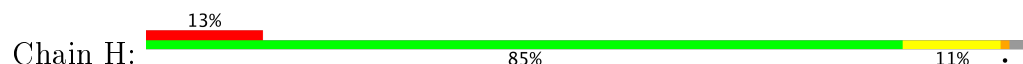
- Molecule 1: Aldoxime dehydratase

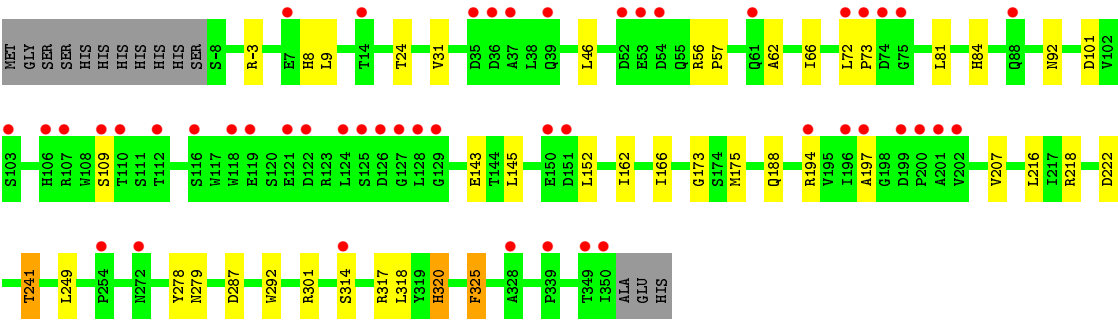


- Molecule 1: Aldoxime dehydratase



- Molecule 1: Aldoxime dehydratase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.05Å 103.93Å 114.19Å 76.50° 89.46° 87.55°	Depositor
Resolution (Å)	19.90 – 2.50 19.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.2 (19.90-2.50) 84.4 (19.90-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.50Å)	Xtriage
Refinement program	REFMAC refmac _5.2.0019	Depositor
R, R_{free}	0.211 , 0.243 0.225 , 0.260	Depositor DCC
R_{free} test set	5656 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23656	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: HEM, BXO

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	0.44	0/2866	0.57	0/3900
1	B	0.42	0/2931	0.57	0/3988
1	C	0.44	0/2891	0.57	0/3934
1	D	0.44	0/2947	0.58	0/4009
1	E	0.43	0/2882	0.58	0/3921
1	F	0.42	0/2931	0.57	0/3988
1	G	0.44	0/2892	0.58	0/3934
1	H	0.42	0/2931	0.56	0/3988
All	All	0.43	0/23271	0.57	0/31662

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	2790	0	2628	25	0
1	B	2853	0	2691	18	0
1	C	2812	0	2652	21	0
1	D	2866	0	2709	30	0
1	E	2803	0	2646	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2853	0	2691	16	0
1	G	2815	0	2646	21	0
1	H	2853	0	2691	21	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	4	0
2	D	43	0	30	1	0
2	E	43	0	30	4	0
2	F	43	0	30	2	0
2	G	43	0	30	4	0
2	H	43	0	30	3	0
3	A	6	0	9	2	0
3	B	6	0	9	1	0
3	C	6	0	9	0	0
3	D	6	0	9	1	0
3	E	6	0	9	0	0
3	F	6	0	9	1	0
3	G	6	0	9	1	0
3	H	6	0	9	3	0
4	A	105	0	0	1	0
4	B	60	0	0	1	0
4	C	93	0	0	0	0
4	D	77	0	0	3	0
4	E	83	0	0	0	0
4	F	58	0	0	0	0
4	G	84	0	0	0	0
4	H	59	0	0	1	0
All	All	23656	0	21666	163	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 (163) 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:D:-3[A]:ARG:HG2	1:D:-3[A]:ARG:HH11	1.41	0.84
1:G:242:LEU:HD22	2:G:354:HEM:HBB1	1.64	0.80
1:E:242:LEU:HD22	2:E:354:HEM:HBB1	1.69	0.75
1:E:305:THR:O	1:E:309:VAL:HG23	1.88	0.73
1:C:242:LEU:HD22	2:C:354:HEM:HBB1	1.70	0.73
1:D:-8:SER:HA	4:D:516:HOH:O	1.89	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:LEU:HD22	2:F:354:HEM:HBB2	1.73	0.70
1:A:29:MET:HE1	3:A:355:B XO:H4	1.74	0.69
1:G:302:ILE:HA	1:G:305:THR:HG23	1.75	0.67
1:E:308:ARG:HE	1:E:309:VAL:HG22	1.58	0.67
1:G:292:TRP:CZ3	2:G:354:HEM:HBC2	2.29	0.67
1:D:-3[A]:ARG:HG2	1:D:-3[A]:ARG:NH1	2.09	0.64
1:B:31:VAL:HG13	1:B:166:ILE:HG12	1.78	0.64
1:A:235:LEU:HB3	1:D:-3[A]:ARG:HD2	1.79	0.63
1:H:318:LEU:HD22	2:H:354:HEM:HBB2	1.79	0.63
1:C:218:ARG:HB3	1:C:321:GLU:HG2	1.80	0.62
1:A:218:ARG:HB3	1:A:321:GLU:HG2	1.80	0.62
1:G:242:LEU:HD22	2:G:354:HEM:CBB	2.30	0.61
1:F:218:ARG:HG3	1:F:278:TYR:CD2	2.36	0.61
1:A:242:LEU:HD22	2:A:354:HEM:HBB1	1.82	0.60
1:H:218:ARG:HG3	1:H:278:TYR:CD2	2.37	0.59
1:A:292:TRP:CZ3	2:A:354:HEM:HBC2	2.37	0.59
1:G:301:ARG:O	1:G:305:THR:HG22	2.04	0.58
1:C:152:LEU:HD21	1:C:162:ILE:HD13	1.85	0.57
1:E:242:LEU:HD22	2:E:354:HEM:CBB	2.35	0.57
1:B:318:LEU:HD22	2:B:354:HEM:HBB2	1.86	0.57
1:G:218:ARG:HB3	1:G:321:GLU:HG2	1.87	0.56
1:E:218:ARG:HB3	1:E:321:GLU:HG2	1.87	0.56
1:A:235:LEU:HB3	1:D:-3[B]:ARG:HD2	1.86	0.56
1:F:31:VAL:HG13	1:F:166:ILE:HG12	1.87	0.56
1:C:150:GLU:N	1:C:150:GLU:OE1	2.37	0.55
1:B:218:ARG:HG3	1:B:278:TYR:CD2	2.42	0.55
1:C:292:TRP:CZ3	2:C:354:HEM:HBC2	2.42	0.55
1:B:81:LEU:N	1:B:81:LEU:HD23	2.22	0.54
1:G:292:TRP:HZ3	2:G:354:HEM:HBC2	1.70	0.54
1:E:292:TRP:CZ3	2:E:354:HEM:HBC2	2.42	0.54
1:H:216:LEU:HB3	1:H:325:PHE:HZ	1.73	0.54
1:H:31:VAL:HG13	1:H:166:ILE:HG12	1.89	0.54
1:B:251:ASP:HB3	1:C:202:VAL:HG21	1.90	0.53
1:B:244:S ER:OG	1:C:351:ALA:HB3	2.07	0.53
1:E:220:GLY:HA3	1:E:319:TYR:CE1	2.44	0.53
1:F:233:LEU:HD21	1:F:309:VAL:HG11	1.91	0.52
1:C:242:LEU:HD22	2:C:354:HEM:CBB	2.38	0.52
1:A:193:LEU:HD11	1:A:343:M ET:HG3	1.92	0.52
1:H:145:LEU:HD23	3:H:355:B XO:C4	2.39	0.52
1:A:152:LEU:HD21	1:A:162:ILE:HD13	1.92	0.52
1:C:287:ASP:O	1:C:291:ARG:HG2	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:VAL:HG11	1:D:105:GLN:HG3	1.91	0.51
1:F:220:GLY:HA3	1:F:319:TYR:CE1	2.46	0.51
1:G:287:ASP:O	1:G:291:ARG:HG2	2.12	0.50
1:D:287:ASP:OD1	1:D:287:ASP:N	2.44	0.50
1:G:42:VAL:HG11	1:G:105:GLN:HG3	1.94	0.50
1:A:292:TRP:HZ3	2:A:354:HEM:HBC2	1.77	0.49
1:B:218:ARG:HA	1:B:279:ASN:O	2.13	0.49
1:F:1:MET:HE3	1:F:165:GLU:HB3	1.94	0.49
1:F:218:ARG:HA	1:F:279:ASN:O	2.12	0.49
1:D:218:ARG:HG3	1:D:278:TYR:CD2	2.48	0.49
1:D:31:VAL:HG13	1:D:166:ILE:HG12	1.93	0.49
1:H:72:LEU:HB3	1:H:73:PRO:HD2	1.95	0.49
1:A:302:ILE:HD12	2:A:354:HEM:HBB2	1.94	0.49
1:D:218:ARG:HA	1:D:279:ASN:O	2.13	0.49
1:F:174:SER:O	1:F:178:ARG:HG3	2.13	0.48
1:H:218:ARG:HA	1:H:279:ASN:O	2.13	0.48
1:E:287:ASP:O	1:E:291:ARG:HG2	2.13	0.48
1:C:220:GLY:HA3	1:C:319:TYR:CE1	2.49	0.47
1:H:145:LEU:HD23	3:H:355:BXO:H4A	1.95	0.47
1:C:117:TRP:O	1:C:123:ARG:NH1	2.47	0.47
1:E:215:ALA:HA	1:E:323:SER:O	2.15	0.47
1:E:302:ILE:HD12	2:E:354:HEM:HBB2	1.96	0.47
1:H:222:ASP:HB3	1:H:317:ARG:HB2	1.96	0.47
1:C:215:ALA:HA	1:C:323:SER:O	2.14	0.47
1:H:84:HIS:CE1	1:H:92:ASN:HB2	2.49	0.47
1:B:287:ASP:N	1:B:287:ASP:OD1	2.44	0.47
1:D:218:ARG:HB3	1:D:321:GLU:HG2	1.96	0.47
1:A:220:GLY:HA3	1:A:319:TYR:CE1	2.50	0.46
1:G:29:MET:HE1	3:G:355:BXO:H4	1.98	0.46
1:D:62:ALA:O	1:D:66:ILE:HG13	2.16	0.46
1:B:222:ASP:HB3	1:B:317:ARG:HB2	1.96	0.46
1:G:152:LEU:HD21	1:G:162:ILE:HD13	1.98	0.46
1:A:215:ALA:HA	1:A:323:SER:O	2.16	0.46
1:B:320:HIS:C	1:B:320:HIS:CD2	2.89	0.46
1:D:222:ASP:HB3	1:D:317:ARG:HB2	1.97	0.46
1:G:215:ALA:HA	1:G:323:SER:O	2.15	0.46
1:H:320:HIS:CD2	1:H:320:HIS:C	2.88	0.46
1:E:218:ARG:HA	1:E:279:ASN:O	2.16	0.46
1:F:152:LEU:HD21	1:F:162:ILE:HD13	1.98	0.46
1:A:29:MET:CE	3:A:355:BXO:H4	2.44	0.45
1:C:211:HIS:CE1	1:C:214:ILE:HG13	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:LEU:HB3	1:F:325:PHE:HZ	1.80	0.45
1:A:236:ASP:OD1	1:D:3[B]:ARG:HD3	2.17	0.45
1:D:84:HIS:CE1	1:D:92:ASN:HB2	2.51	0.45
1:F:193:LEU:O	1:F:348:VAL:HG12	2.17	0.45
1:F:218:ARG:HB3	1:F:321:GLU:HG2	1.99	0.44
1:A:287:ASP:O	1:A:291:ARG:HG2	2.16	0.44
1:D:143:GLU:OE2	1:D:175:MET:HG3	2.18	0.44
1:G:220:GLY:HA3	1:G:319:TYR:CE1	2.53	0.44
1:H:249:LEU:HD21	1:H:292:TRP:CE2	2.52	0.44
1:D:11:CYS:HB2	1:D:12:PRO:HD2	1.99	0.44
1:E:308:ARG:NE	1:E:309:VAL:HG22	2.31	0.44
1:G:150:GLU:OE1	1:G:150:GLU:N	2.49	0.44
1:G:218:ARG:HA	1:G:279:ASN:O	2.18	0.44
1:G:47:GLY:HA3	1:G:131:PHE:CZ	2.53	0.44
1:A:145:LEU:HD22	1:A:178:ARG:NH2	2.33	0.44
1:B:216:LEU:HB3	1:B:325:PHE:HZ	1.83	0.44
1:D:39:GLN:HG2	4:D:514:HOH:O	2.17	0.44
1:A:186:TRP:HH2	1:B:17:ARG:O	1.99	0.43
1:B:218:ARG:HB3	1:B:321:GLU:HG2	2.00	0.43
1:H:173:GLY:HA2	4:H:374:HOH:O	2.18	0.43
1:E:18:ARG:HD2	1:F:18:ARG:HD2	2.00	0.43
1:A:194:ARG:HG2	1:A:348:VAL:CG2	2.49	0.43
1:C:17:ARG:O	1:D:186:TRP:HH2	2.01	0.43
1:F:81:LEU:HD23	1:F:81:LEU:N	2.33	0.43
1:G:196:ILE:HD13	1:G:209:ARG:HB2	2.00	0.43
1:C:233:LEU:HA	1:C:237:GLU:HG3	2.01	0.43
1:G:145:LEU:HD22	1:G:178:ARG:NH2	2.34	0.43
1:G:56:ARG:HB3	1:G:57:PRO:HD3	2.00	0.43
1:A:132:ARG:HG2	1:A:333:GLU:HB2	2.01	0.42
1:B:84:HIS:CE1	1:B:92:ASN:HB2	2.54	0.42
1:D:320:HIS:C	1:D:320:HIS:CD2	2.92	0.42
1:F:62:ALA:O	1:F:66:ILE:HG13	2.19	0.42
1:C:241:THR:HG21	1:C:301:ARG:HB3	2.01	0.42
1:C:218:ARG:HA	1:C:279:ASN:O	2.19	0.42
1:E:56:ARG:HB3	1:E:57:PRO:HD3	2.00	0.42
1:B:173:GLY:HA2	4:B:367:HOH:O	2.20	0.42
1:D:152:LEU:HD21	1:D:162:ILE:HD13	2.01	0.42
1:A:218:ARG:HA	1:A:279:ASN:O	2.19	0.42
1:D:11:CYS:HB2	1:D:12:PRO:CD	2.49	0.41
1:D:24:THR:HA	1:D:25:PRO:HD3	1.95	0.41
1:A:56:ARG:HB3	1:A:57:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:VAL:HG11	1:C:105:GLN:HG3	2.02	0.41
1:C:18:ARG:HD2	1:D:18:ARG:HD2	2.01	0.41
1:H:143:GLU:OE2	1:H:175:MET:HG3	2.20	0.41
1:C:302:ILE:HD12	2:C:354:HEM:HBB2	2.02	0.41
1:E:152:LEU:HD21	1:E:162:ILE:HD13	2.02	0.41
1:C:76:PRO:HD3	1:C:99:TRP:CZ2	2.55	0.41
1:D:216:LEU:HB3	1:D:325:PHE:HZ	1.86	0.41
1:H:62:ALA:O	1:H:66:ILE:HG13	2.20	0.41
1:A:209:ARG:NE	4:A:588:HOH:O	2.52	0.41
1:D:218:ARG:HB3	1:D:321:GLU:CG	2.50	0.41
2:D:354:HEM:C4A	3:D:355:BXO:H1	2.56	0.41
1:E:47:GLY:HA3	1:E:131:PHE:CZ	2.56	0.41
1:F:258:CYS:SG	1:F:261:ASN:HB2	2.61	0.41
1:A:254:PRO:HD3	1:A:345:ARG:NH2	2.36	0.41
1:D:1:MET:HE2	1:D:25:PRO:HG2	2.02	0.41
1:H:152:LEU:HD21	1:H:162:ILE:HD13	2.02	0.41
2:B:354:HEM:C4A	3:B:355:BXO:H1	2.56	0.41
1:H:241:THR:HG21	1:H:301:ARG:HD3	2.03	0.41
1:A:123:ARG:HD3	1:A:123:ARG:HA	1.92	0.41
1:B:8:HIS:CE1	1:B:9:LEU:HG	2.56	0.41
1:H:197:ALA:HB3	1:H:207:VAL:HB	2.03	0.41
1:H:56:ARG:HB3	1:H:57:PRO:HD3	2.03	0.41
1:B:258:CYS:SG	1:B:261:ASN:HB2	2.61	0.41
1:D:12:PRO:HD3	4:D:598:HOH:O	2.20	0.41
1:D:1:MET:HE3	1:D:165:GLU:HB3	2.03	0.40
1:B:152:LEU:HD21	1:B:162:ILE:HD13	2.02	0.40
2:H:354:HEM:C4A	3:H:355:BXO:H1	2.56	0.40
1:A:196:ILE:HD13	1:A:209:ARG:HB2	2.02	0.40
1:D:64:ARG:HG2	1:D:269:ILE:HD11	2.04	0.40
1:G:284:ALA:HB3	1:G:288:GLN:HE22	1.87	0.40
1:H:279:ASN:OD1	2:H:354:HEM:HAC	2.22	0.40
2:F:354:HEM:C4A	3:F:355:BXO:H1	2.56	0.40
1:G:241:THR:OG1	1:G:302:ILE:HG23	2.22	0.40
1:H:8:HIS:CE1	1:H:9:LEU:HG	2.56	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	348/373 (93%)	346 (99%)	2 (1%)	0	100	100
1	B	357/373 (96%)	354 (99%)	3 (1%)	0	100	100
1	C	351/373 (94%)	346 (99%)	5 (1%)	0	100	100
1	D	359/373 (96%)	357 (99%)	2 (1%)	0	100	100
1	E	350/373 (94%)	346 (99%)	4 (1%)	0	100	100
1	F	357/373 (96%)	354 (99%)	3 (1%)	0	100	100
1	G	351/373 (94%)	347 (99%)	4 (1%)	0	100	100
1	H	357/373 (96%)	357 (100%)	0	0	100	100
All	All	2830/2984 (95%)	2807 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	293/312 (94%)	285 (97%)	8 (3%)	50	77
1	B	300/312 (96%)	289 (96%)	11 (4%)	39	66
1	C	295/312 (95%)	283 (96%)	12 (4%)	35	61
1	D	301/312 (96%)	287 (95%)	14 (5%)	30	54
1	E	294/312 (94%)	288 (98%)	6 (2%)	60	84
1	F	300/312 (96%)	286 (95%)	14 (5%)	30	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	295/312 (95%)	287 (97%)	8 (3%)	50	77
1	H	300/312 (96%)	287 (96%)	13 (4%)	33	58
All	All	2378/2496 (95%)	2292 (96%)	86 (4%)	40	67

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	LEU
1	A	109	SER
1	A	123	ARG
1	A	150	GLU
1	A	320	HIS
1	A	325	PHE
1	A	343	MET
1	A	349	THR
1	B	81	LEU
1	B	101	ASP
1	B	109	SER
1	B	150	GLU
1	B	241	THR
1	B	287	ASP
1	B	301	ARG
1	B	308	ARG
1	B	315	LYS
1	B	320	HIS
1	B	325	PHE
1	C	53	GLU
1	C	81	LEU
1	C	105	GLN
1	C	150	GLU
1	C	237	GLU
1	C	309	VAL
1	C	320	HIS
1	C	325	PHE
1	C	343	MET
1	C	348	VAL
1	C	350	ILE
1	C	352	GLU
1	D	-3[A]	ARG
1	D	-3[B]	ARG
1	D	24	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	38	LEU
1	D	46	LEU
1	D	81	LEU
1	D	101	ASP
1	D	105	GLN
1	D	109	SER
1	D	150	GLU
1	D	287	ASP
1	D	314	SER
1	D	320	HIS
1	D	325	PHE
1	E	81	LEU
1	E	193	LEU
1	E	309	VAL
1	E	320	HIS
1	E	325	PHE
1	E	350	ILE
1	F	-3	ARG
1	F	24	THR
1	F	46	LEU
1	F	81	LEU
1	F	101	ASP
1	F	109	SER
1	F	150	GLU
1	F	241	THR
1	F	287	ASP
1	F	314	SER
1	F	315	LYS
1	F	320	HIS
1	F	325	PHE
1	F	349	THR
1	G	81	LEU
1	G	123	ARG
1	G	287	ASP
1	G	305	THR
1	G	320	HIS
1	G	325	PHE
1	G	343	MET
1	G	348	VAL
1	H	-3	ARG
1	H	24	THR
1	H	46	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	81	LEU
1	H	101	ASP
1	H	109	SER
1	H	188	GLN
1	H	194	ARG
1	H	241	THR
1	H	287	ASP
1	H	314	SER
1	H	320	HIS
1	H	325	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	GLN
1	B	105	GLN
1	C	288	GLN
1	D	105	GLN
1	E	105	GLN
1	E	288	GLN
1	F	105	GLN
1	G	105	GLN
1	G	288	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

16 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	HEM	A	354	1,3	28,50,50	2.11	6 (21%)	17,82,82	1.88	4 (23%)
3	BXO	A	355	2	4,5,5	0.50	0	3,4,4	6.17	2 (66%)
2	HEM	B	354	1,3	28,50,50	2.27	10 (35%)	17,82,82	1.31	2 (11%)
3	BXO	B	355	2	4,5,5	1.13	1 (25%)	3,4,4	4.41	2 (66%)
2	HEM	C	354	1,3	28,50,50	2.12	6 (21%)	17,82,82	1.86	4 (23%)
3	BXO	C	355	2	4,5,5	1.34	1 (25%)	3,4,4	4.71	2 (66%)
2	HEM	D	354	1,3	28,50,50	2.20	9 (32%)	17,82,82	1.33	2 (11%)
3	BXO	D	355	2	4,5,5	1.17	1 (25%)	3,4,4	4.21	2 (66%)
2	HEM	E	354	1,3	28,50,50	2.16	7 (25%)	17,82,82	1.81	3 (17%)
3	BXO	E	355	2	4,5,5	1.31	1 (25%)	3,4,4	4.20	2 (66%)
2	HEM	F	354	1,3	28,50,50	2.21	10 (35%)	17,82,82	1.29	1 (5%)
3	BXO	F	355	2	4,5,5	1.10	1 (25%)	3,4,4	4.22	2 (66%)
2	HEM	G	354	1,3	28,50,50	2.10	5 (17%)	17,82,82	1.84	4 (23%)
3	BXO	G	355	2	4,5,5	1.39	1 (25%)	3,4,4	4.18	2 (66%)
2	HEM	H	354	1,3	28,50,50	2.21	8 (28%)	17,82,82	1.30	2 (11%)
3	BXO	H	355	2	4,5,5	0.96	0	3,4,4	4.34	2 (66%)

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	HEM	A	354	1,3	-	0/6/54/54	0/0/8/8
3	BXO	A	355	2	-	0/2/3/3	0/0/0/0
2	HEM	B	354	1,3	-	0/6/54/54	0/0/8/8
3	BXO	B	355	2	-	0/2/3/3	0/0/0/0
2	HEM	C	354	1,3	-	0/6/54/54	0/0/8/8
3	BXO	C	355	2	-	0/2/3/3	0/0/0/0
2	HEM	D	354	1,3	-	0/6/54/54	0/0/8/8
3	BXO	D	355	2	-	0/2/3/3	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	E	354	1,3	-	0/6/54/54	0/0/8/8
3	BXO	E	355	2	-	0/2/3/3	0/0/0/0
2	HEM	F	354	1,3	-	0/6/54/54	0/0/8/8
3	BXO	F	355	2	-	0/2/3/3	0/0/0/0
2	HEM	G	354	1,3	-	0/6/54/54	0/0/8/8
3	BXO	G	355	2	-	0/2/3/3	0/0/0/0
2	HEM	H	354	1,3	-	0/6/54/54	0/0/8/8
3	BXO	H	355	2	-	0/2/3/3	0/0/0/0

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	354	HEM	C3B-C2B	-5.04	1.33	1.40
2	H	354	HEM	C3B-C2B	-4.81	1.34	1.40
2	E	354	HEM	C3C-C2C	-4.76	1.34	1.40
2	F	354	HEM	C3B-C2B	-4.75	1.34	1.40
2	D	354	HEM	C3B-C2B	-4.66	1.34	1.40
2	C	354	HEM	C3C-C2C	-4.63	1.34	1.40
2	G	354	HEM	C3C-C2C	-4.58	1.34	1.40
2	A	354	HEM	C3C-C2C	-4.57	1.34	1.40
2	E	354	HEM	C3B-C2B	-4.44	1.34	1.40
2	D	354	HEM	C3C-C2C	-4.33	1.34	1.40
2	B	354	HEM	C3C-C2C	-4.23	1.34	1.40
2	G	354	HEM	C3B-C2B	-4.23	1.34	1.40
2	F	354	HEM	C3C-C2C	-4.09	1.34	1.40
2	H	354	HEM	C3C-C2C	-4.09	1.35	1.40
2	C	354	HEM	C3B-C2B	-4.01	1.35	1.40
2	A	354	HEM	C3B-C2B	-3.95	1.35	1.40
2	D	354	HEM	CMC-C2C	2.03	1.55	1.51
2	B	354	HEM	CAA-C2A	2.04	1.55	1.52
2	D	354	HEM	C1B-NB	2.04	1.39	1.36
2	F	354	HEM	CMC-C2C	2.04	1.55	1.51
2	E	354	HEM	CMA-C3A	2.06	1.55	1.51
2	B	354	HEM	CMB-C2B	2.07	1.56	1.51
3	B	355	BXO	C1-N1	2.07	1.28	1.26
2	F	354	HEM	CMB-C2B	2.08	1.56	1.51
2	F	354	HEM	CMA-C3A	2.11	1.55	1.51
2	D	354	HEM	CAD-C3D	2.13	1.56	1.52
2	C	354	HEM	C4D-ND	2.14	1.39	1.36
2	H	354	HEM	CMB-C2B	2.15	1.56	1.51
3	F	355	BXO	C1-N1	2.16	1.28	1.26
2	H	354	HEM	CAD-C3D	2.17	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	354	HEM	CAD-C3D	2.22	1.56	1.52
3	D	355	BXO	C1-N1	2.27	1.28	1.26
2	A	354	HEM	C4D-ND	2.28	1.39	1.36
2	H	354	HEM	C4D-ND	2.28	1.39	1.36
2	B	354	HEM	CAD-C3D	2.29	1.56	1.52
2	F	354	HEM	C4D-ND	2.31	1.39	1.36
2	B	354	HEM	CMC-C2C	2.41	1.56	1.51
2	D	354	HEM	C4D-ND	2.42	1.39	1.36
2	B	354	HEM	C4D-ND	2.52	1.39	1.36
3	E	355	BXO	C1-N1	2.56	1.28	1.26
2	E	354	HEM	C4D-ND	2.60	1.39	1.36
3	C	355	BXO	C1-N1	2.63	1.28	1.26
3	G	355	BXO	C1-N1	2.74	1.28	1.26
2	G	354	HEM	C3C-CAC	3.03	1.53	1.47
2	E	354	HEM	C3C-CAC	3.22	1.54	1.47
2	A	354	HEM	C3C-CAC	3.25	1.54	1.47
2	C	354	HEM	C3C-CAC	3.29	1.54	1.47
2	C	354	HEM	C3B-CAB	3.51	1.54	1.47
2	G	354	HEM	C3B-CAB	3.59	1.55	1.47
2	F	354	HEM	C3B-CAB	3.59	1.55	1.47
2	H	354	HEM	C3B-CAB	3.65	1.55	1.47
2	A	354	HEM	C3B-CAB	3.65	1.55	1.47
2	E	354	HEM	C3B-CAB	3.71	1.55	1.47
2	D	354	HEM	C3B-CAB	3.77	1.55	1.47
2	D	354	HEM	C3C-CAC	3.79	1.55	1.47
2	B	354	HEM	C3C-CAC	3.82	1.55	1.47
2	B	354	HEM	C3B-CAB	4.00	1.55	1.47
2	H	354	HEM	C3C-CAC	4.01	1.55	1.47
2	F	354	HEM	C3C-CAC	4.13	1.55	1.47
2	D	354	HEM	C3D-C2D	4.84	1.52	1.37
2	H	354	HEM	C3D-C2D	4.91	1.52	1.37
2	F	354	HEM	C3D-C2D	5.00	1.52	1.37
2	B	354	HEM	C3D-C2D	5.00	1.52	1.37
2	A	354	HEM	C3D-C2D	5.04	1.52	1.37
2	G	354	HEM	C3D-C2D	5.10	1.52	1.37
2	C	354	HEM	C3D-C2D	5.16	1.52	1.37
2	E	354	HEM	C3D-C2D	5.17	1.53	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	354	HEM	CBA-CAA-C2A	-5.06	102.81	112.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	354	HEM	CBA-CAA-C2A	-5.03	102.88	112.48
2	E	354	HEM	CBA-CAA-C2A	-4.96	102.99	112.48
2	G	354	HEM	CBA-CAA-C2A	-4.92	103.07	112.48
3	F	355	BXO	C3-C2-C1	-4.72	107.72	112.88
3	H	355	BXO	C3-C2-C1	-4.61	107.84	112.88
3	B	355	BXO	C3-C2-C1	-4.34	108.14	112.88
3	D	355	BXO	C3-C2-C1	-4.09	108.41	112.88
2	D	354	HEM	CAA-CBA-CGA	-3.49	106.69	112.66
2	F	354	HEM	CAA-CBA-CGA	-3.28	107.05	112.66
2	H	354	HEM	CAA-CBA-CGA	-3.07	107.42	112.66
2	B	354	HEM	CAA-CBA-CGA	-3.05	107.44	112.66
2	A	354	HEM	CAD-CBD-CGD	-3.01	107.51	112.66
3	A	355	BXO	C3-C2-C1	-2.98	109.62	112.88
2	G	354	HEM	CAD-CBD-CGD	-2.93	107.65	112.66
2	C	354	HEM	CAD-CBD-CGD	-2.84	107.81	112.66
3	G	355	BXO	C3-C2-C1	-2.78	109.84	112.88
2	E	354	HEM	CAD-CBD-CGD	-2.70	108.05	112.66
2	G	354	HEM	C1D-C2D-C3D	-2.50	105.26	107.00
3	E	355	BXO	C3-C2-C1	-2.49	110.17	112.88
2	C	354	HEM	C1D-C2D-C3D	-2.45	105.29	107.00
2	E	354	HEM	C1D-C2D-C3D	-2.32	105.38	107.00
3	C	355	BXO	C3-C2-C1	-2.29	110.38	112.88
2	A	354	HEM	C1D-C2D-C3D	-2.23	105.44	107.00
2	B	354	HEM	CMA-C3A-C4A	-2.02	125.36	128.46
2	D	354	HEM	CMA-C3A-C4A	-2.01	125.37	128.46
2	H	354	HEM	CMA-C3A-C4A	-2.00	125.39	128.46
2	C	354	HEM	C4C-C3C-C2C	2.14	108.39	106.90
2	G	354	HEM	C4C-C3C-C2C	2.23	108.45	106.90
2	A	354	HEM	C4C-C3C-C2C	2.26	108.48	106.90
3	F	355	BXO	O1-N1-C1	5.57	117.05	111.69
3	H	355	BXO	O1-N1-C1	5.93	117.39	111.69
3	D	355	BXO	O1-N1-C1	6.02	117.48	111.69
3	B	355	BXO	O1-N1-C1	6.29	117.74	111.69
3	G	355	BXO	O1-N1-C1	6.69	118.12	111.69
3	E	355	BXO	O1-N1-C1	6.83	118.26	111.69
3	C	355	BXO	O1-N1-C1	7.84	119.22	111.69
3	A	355	BXO	O1-N1-C1	10.26	121.55	111.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	354	HEM	4	0
3	A	355	BXO	2	0
2	B	354	HEM	2	0
3	B	355	BXO	1	0
2	C	354	HEM	4	0
2	D	354	HEM	1	0
3	D	355	BXO	1	0
2	E	354	HEM	4	0
2	F	354	HEM	2	0
3	F	355	BXO	1	0
2	G	354	HEM	4	0
3	G	355	BXO	1	0
2	H	354	HEM	3	0
3	H	355	BXO	3	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 ⓘ

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	350/373 (93%)	0.36	17 (4%) 30 32	13, 25, 39, 55	0
1	B	359/373 (96%)	0.67	42 (11%) 5 4	15, 31, 57, 67	0
1	C	352/373 (94%)	0.38	23 (6%) 20 20	14, 25, 40, 55	0
1	D	360/373 (96%)	0.63	37 (10%) 7 6	15, 31, 57, 68	0
1	E	351/373 (94%)	0.37	27 (7%) 14 14	14, 25, 40, 55	0
1	F	359/373 (96%)	0.65	43 (11%) 5 4	15, 31, 57, 68	0
1	G	353/373 (94%)	0.39	23 (6%) 20 20	13, 25, 41, 55	0
1	H	359/373 (96%)	0.62	48 (13%) 4 3	15, 31, 57, 68	0
All	All	2843/2984 (95%)	0.51	260 (9%) 10 10	13, 26, 55, 68	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	353	HIS	7.7
1	G	351	ALA	6.8
1	H	350	ILE	6.8
1	F	201	ALA	6.7
1	D	350	ILE	6.6
1	F	350	ILE	6.2
1	B	126	ASP	6.1
1	F	125	SER	6.0
1	H	75	GLY	6.0
1	C	351	ALA	5.9
1	E	124	LEU	5.9
1	B	201	ALA	5.8
1	F	126	ASP	5.7
1	E	12	PRO	5.6
1	G	121	GLU	5.5
1	A	124	LEU	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	350	ILE	5.3
1	D	112	THR	5.3
1	F	110	THR	5.1
1	C	12	PRO	5.1
1	G	12	PRO	5.0
1	F	127	GLY	5.0
1	B	125	SER	4.8
1	F	121	GLU	4.8
1	B	103	SER	4.8
1	B	112	THR	4.8
1	H	201	ALA	4.7
1	E	125	SER	4.7
1	A	12	PRO	4.6
1	A	125	SER	4.6
1	E	351	ALA	4.6
1	C	311	ALA	4.5
1	H	202	VAL	4.5
1	D	-8	SER	4.5
1	D	106	HIS	4.4
1	H	121	GLU	4.4
1	C	125	SER	4.3
1	C	124	LEU	4.3
1	F	122	ASP	4.2
1	B	194	ARG	4.1
1	B	121	GLU	4.1
1	D	113	PRO	4.1
1	H	106	HIS	4.0
1	H	126	ASP	3.9
1	G	124	LEU	3.9
1	B	54	ASP	3.8
1	H	122	ASP	3.8
1	D	351	ALA	3.8
1	H	103	SER	3.8
1	H	127	GLY	3.8
1	E	51	ARG	3.7
1	E	21	ASP	3.7
1	F	74	ASP	3.6
1	D	125	SER	3.6
1	A	121	GLU	3.6
1	H	125	SER	3.6
1	E	121	GLU	3.6
1	F	12	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	112	THR	3.6
1	D	201	ALA	3.6
1	D	122	ASP	3.5
1	F	106	HIS	3.5
1	B	63	MET	3.5
1	F	119	GLU	3.5
1	D	150	GLU	3.5
1	B	53	GLU	3.5
1	F	349	THR	3.5
1	E	311	ALA	3.4
1	A	36	ASP	3.4
1	B	73	PRO	3.4
1	F	54	ASP	3.4
1	D	349	THR	3.3
1	F	103	SER	3.3
1	G	125	SER	3.3
1	F	52	ASP	3.3
1	H	194	ARG	3.3
1	B	122	ASP	3.3
1	G	126	ASP	3.3
1	C	318	LEU	3.2
1	A	123	ARG	3.2
1	D	121	GLU	3.2
1	H	53	GLU	3.2
1	F	112	THR	3.2
1	F	-8	SER	3.2
1	F	328	ALA	3.2
1	D	73	PRO	3.2
1	D	119	GLU	3.1
1	C	36	ASP	3.1
1	H	349	THR	3.1
1	F	111	SER	3.1
1	D	110	THR	3.1
1	B	205	ARG	3.1
1	F	73	PRO	3.0
1	E	150	GLU	3.0
1	A	311	ALA	3.0
1	H	119	GLU	3.0
1	H	112	THR	3.0
1	D	53	GLU	3.0
1	D	36	ASP	3.0
1	B	116	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	112	THR	3.0
1	B	12	PRO	3.0
1	E	126	ASP	2.9
1	E	1	MET	2.9
1	G	1	MET	2.9
1	D	75	GLY	2.9
1	B	52	ASP	2.9
1	B	349	THR	2.9
1	D	72	LEU	2.9
1	G	22	THR	2.9
1	B	119	GLU	2.8
1	G	54	ASP	2.8
1	H	52	ASP	2.8
1	H	54	ASP	2.8
1	H	328	ALA	2.8
1	H	73	PRO	2.8
1	F	196	ILE	2.7
1	H	36	ASP	2.7
1	B	72	LEU	2.7
1	G	123	ARG	2.7
1	G	36	ASP	2.7
1	F	113	PRO	2.7
1	D	126	ASP	2.7
1	B	269	ILE	2.7
1	B	7	GLU	2.7
1	A	54	ASP	2.7
1	F	7	GLU	2.7
1	F	151	ASP	2.7
1	H	110	THR	2.6
1	F	35	ASP	2.6
1	F	53	GLU	2.6
1	B	202	VAL	2.6
1	A	318	LEU	2.6
1	G	318	LEU	2.6
1	E	53	GLU	2.6
1	H	61	GLN	2.6
1	C	54	ASP	2.6
1	F	194	ARG	2.6
1	B	128	LEU	2.6
1	F	336	ASN	2.6
1	H	151	ASP	2.6
1	H	254	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	35	ASP	2.6
1	F	51	ARG	2.6
1	F	348	VAL	2.6
1	A	116	SER	2.6
1	B	272	ASN	2.6
1	D	7	GLU	2.6
1	B	71	ASP	2.5
1	F	118	TRP	2.5
1	F	347	ALA	2.5
1	H	200	PRO	2.5
1	H	107	ARG	2.5
1	E	350	ILE	2.5
1	C	122	ASP	2.5
1	F	75	GLY	2.5
1	G	116	SER	2.5
1	D	328	ALA	2.5
1	D	339	PRO	2.5
1	E	318	LEU	2.5
1	F	128	LEU	2.5
1	C	11	CYS	2.5
1	G	53	GLU	2.5
1	G	311	ALA	2.5
1	A	21	ASP	2.5
1	H	199	ASP	2.5
1	B	348	VAL	2.5
1	F	205	ARG	2.5
1	C	126	ASP	2.5
1	D	54	ASP	2.5
1	C	110	THR	2.5
1	E	122	ASP	2.4
1	B	328	ALA	2.4
1	B	190	SER	2.4
1	H	150	GLU	2.4
1	H	124	LEU	2.4
1	D	131	PHE	2.4
1	D	194	ARG	2.4
1	H	339	PRO	2.4
1	C	192	GLU	2.4
1	B	36	ASP	2.4
1	B	-8	SER	2.4
1	B	127	GLY	2.4
1	F	0	HIS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	118	TRP	2.4
1	B	336	ASN	2.3
1	C	51	ARG	2.3
1	C	123	ARG	2.3
1	E	194	ARG	2.3
1	G	21	ASP	2.3
1	D	14	THR	2.3
1	B	75	GLY	2.3
1	H	116	SER	2.3
1	C	121	GLU	2.3
1	C	57	PRO	2.3
1	B	151	ASP	2.3
1	A	51	ARG	2.3
1	G	314	SER	2.3
1	E	36	ASP	2.3
1	D	12	PRO	2.3
1	C	1	MET	2.3
1	H	272	ASN	2.3
1	D	124	LEU	2.3
1	D	48	VAL	2.2
1	H	35	ASP	2.2
1	A	53	GLU	2.2
1	B	110	THR	2.2
1	B	118	TRP	2.2
1	F	72	LEU	2.2
1	C	53	GLU	2.2
1	G	51	ARG	2.2
1	B	117	TRP	2.2
1	E	308	ARG	2.2
1	H	197	ALA	2.2
1	H	14	THR	2.2
1	H	196	ILE	2.2
1	H	128	LEU	2.2
1	D	327	ALA	2.2
1	E	269	ILE	2.2
1	D	151	ASP	2.2
1	D	202	VAL	2.2
1	F	272	ASN	2.2
1	G	122	ASP	2.2
1	H	74	ASP	2.2
1	E	11	CYS	2.2
1	D	190	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	350	ILE	2.1
1	H	39	GLN	2.1
1	B	48	VAL	2.1
1	G	352	GLU	2.1
1	C	71	ASP	2.1
1	C	301	ARG	2.1
1	E	205	ARG	2.1
1	B	47	GLY	2.1
1	H	129	GLY	2.1
1	F	197	ALA	2.1
1	A	349	THR	2.1
1	H	7	GLU	2.1
1	E	314	SER	2.1
1	H	72	LEU	2.1
1	E	192	GLU	2.1
1	E	123	ARG	2.1
1	F	202	VAL	2.1
1	G	151	ASP	2.1
1	H	314	SER	2.1
1	D	39	GLN	2.1
1	F	192	GLU	2.1
1	F	36	ASP	2.0
1	G	225	ASP	2.0
1	H	37	ALA	2.0
1	C	112	THR	2.0
1	E	7	GLU	2.0
1	A	194	ARG	2.0
1	D	118	TRP	2.0
1	B	62	ALA	2.0
1	B	68	ALA	2.0
1	E	224	ALA	2.0
1	H	88	GLN	2.0
1	H	109	SER	2.0
1	A	71	ASP	2.0

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

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(Å ²)	Q<0.9
3	BXO	D	355	6/6	0.94	0.22	1.72	25,26,27,28	0
3	BXO	B	355	6/6	0.93	0.21	1.65	25,26,27,28	0
3	BXO	F	355	6/6	0.93	0.17	0.17	25,26,27,28	0
3	BXO	G	355	6/6	0.95	0.19	0.13	18,20,21,21	0
3	BXO	H	355	6/6	0.97	0.16	-0.02	25,26,27,28	0
3	BXO	E	355	6/6	0.96	0.17	-0.07	18,20,21,21	0
3	BXO	A	355	6/6	0.97	0.19	-0.11	18,20,21,21	0
2	HEM	H	354	43/43	0.96	0.15	-0.20	12,13,17,17	0
2	HEM	D	354	43/43	0.95	0.16	-0.23	12,13,17,17	0
3	BXO	C	355	6/6	0.98	0.17	-0.32	18,20,21,21	0
2	HEM	E	354	43/43	0.96	0.15	-0.49	13,15,18,18	0
2	HEM	F	354	43/43	0.96	0.14	-0.63	12,13,17,17	0
2	HEM	B	354	43/43	0.96	0.14	-0.65	12,13,17,17	0
2	HEM	G	354	43/43	0.97	0.13	-0.80	13,15,18,18	0
2	HEM	A	354	43/43	0.97	0.14	-0.90	13,15,18,18	0
2	HEM	C	354	43/43	0.97	0.12	-1.18	13,15,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.