



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:12 PM UTC

PDB ID : 1IES / pdb_00001ies
Title : TETRAGONAL CRYSTAL STRUCTURE OF NATIVE HORSE SPLEEN FERRITIN
Authors : Granier, T.; Gallois, B.; Dautant, A.; Langlois D'Estaintot, B.; Precigoux, G.
Deposited on : 1996-05-28
Resolution : 2.60 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

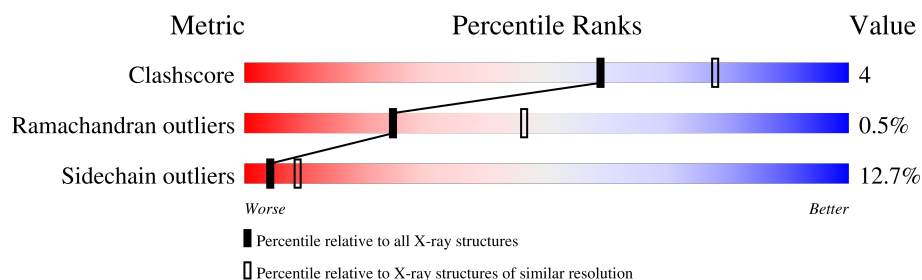
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	174	
1	B	174	
1	C	174	
1	D	174	
1	E	174	
1	F	174	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8665 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 FERRITIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1398	879	246	268	5			
1	B	174	Total	C	N	O	S	0	0	0
			1398	879	246	268	5			
1	C	174	Total	C	N	O	S	0	0	0
			1398	879	246	268	5			
1	D	174	Total	C	N	O	S	0	0	0
			1398	879	246	268	5			
1	E	174	Total	C	N	O	S	0	0	0
			1398	879	246	268	5			
1	F	174	Total	C	N	O	S	0	0	0
			1398	879	246	268	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	LEU	PRO	conflict	UNP P02791
B	93	LEU	PRO	conflict	UNP P02791
C	93	LEU	PRO	conflict	UNP P02791
D	93	LEU	PRO	conflict	UNP P02791
E	93	LEU	PRO	conflict	UNP P02791
F	93	LEU	PRO	conflict	UNP P02791

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		
2	B	2	Total	Cd	0	0
			2	2		
2	D	2	Total	Cd	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	52	Total 52	O 52	0	0
3	C	49	Total 49	O 49	0	0
3	D	38	Total 38	O 38	0	0
3	E	39	Total 39	O 39	0	0
3	F	43	Total 43	O 43	0	0

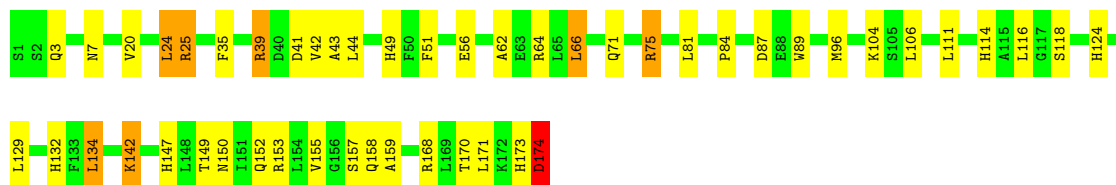
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

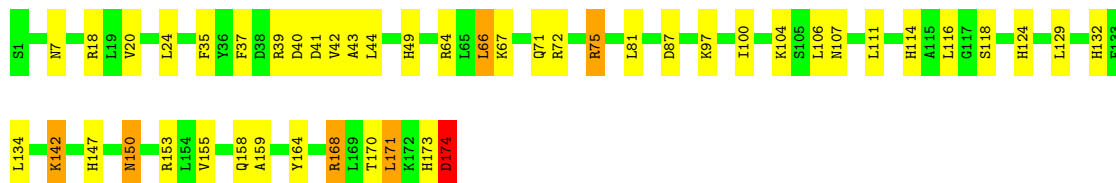
• Molecule 1: FERRITIN

Chain A: 



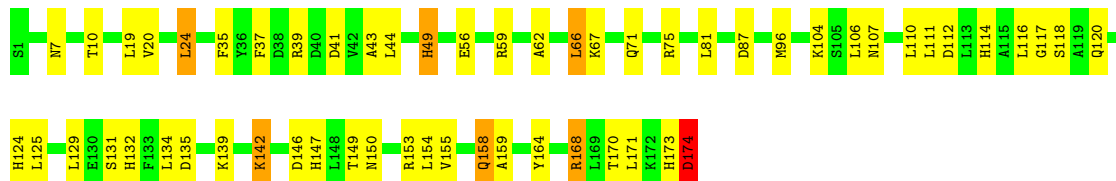
• Molecule 1: FERRITIN

Chain B: 



• Molecule 1: FERRITIN

Chain C: 



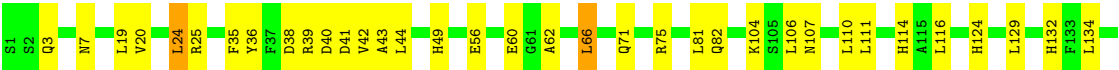
• Molecule 1: FERRITIN

Chain D: 





• Molecule 1: FERRITIN



• Molecule 1: FERRITIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	147.23Å 147.23Å 152.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.60)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 2.1	Depositor
R, R_{free}	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8665	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.11	7/1421 (0.5%)	1.67	23/1911 (1.2%)
1	B	1.10	5/1421 (0.4%)	1.66	19/1911 (1.0%)
1	C	1.13	6/1421 (0.4%)	1.70	27/1911 (1.4%)
1	D	1.04	6/1421 (0.4%)	1.70	21/1911 (1.1%)
1	E	1.08	8/1421 (0.6%)	1.60	16/1911 (0.8%)
1	F	1.03	5/1421 (0.4%)	1.59	16/1911 (0.8%)
All	All	1.08	37/8526 (0.4%)	1.66	122/11466 (1.1%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	HIS	CD2-NE2	-7.19	1.29	1.37
1	E	147	HIS	CD2-NE2	-6.79	1.30	1.37
1	A	124	HIS	CD2-NE2	-6.52	1.30	1.37
1	C	147	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	147	HIS	CD2-NE2	-6.49	1.30	1.37
1	D	124	HIS	CD2-NE2	-6.47	1.30	1.37
1	E	124	HIS	CD2-NE2	-6.41	1.30	1.37
1	C	173	HIS	CD2-NE2	-6.32	1.30	1.37
1	B	173	HIS	CD2-NE2	-6.32	1.30	1.37
1	A	173	HIS	CD2-NE2	-6.28	1.30	1.37
1	F	173	HIS	CD2-NE2	-6.28	1.30	1.37
1	C	124	HIS	CD2-NE2	-6.26	1.30	1.37
1	E	173	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	132	HIS	CD2-NE2	-6.23	1.30	1.37
1	D	173	HIS	CD2-NE2	-6.22	1.31	1.37
1	B	124	HIS	CD2-NE2	-6.18	1.31	1.37
1	F	132	HIS	CD2-NE2	-6.18	1.31	1.37
1	D	132	HIS	CD2-NE2	-6.18	1.31	1.37
1	E	114	HIS	CD2-NE2	-6.17	1.31	1.37
1	F	49	HIS	CD2-NE2	-6.15	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	HIS	CD2-NE2	-6.08	1.31	1.37
1	C	49	HIS	CD2-NE2	-6.06	1.31	1.37
1	F	124	HIS	CD2-NE2	-5.99	1.31	1.37
1	A	132	HIS	CD2-NE2	-5.94	1.31	1.37
1	E	132	HIS	CD2-NE2	-5.92	1.31	1.37
1	C	132	HIS	CD2-NE2	-5.88	1.31	1.37
1	B	114	HIS	CD2-NE2	-5.87	1.31	1.37
1	F	114	HIS	CD2-NE2	-5.83	1.31	1.37
1	A	114	HIS	CD2-NE2	-5.55	1.31	1.37
1	D	49	HIS	CD2-NE2	-5.52	1.31	1.37
1	C	114	HIS	CD2-NE2	-5.43	1.31	1.37
1	A	49	HIS	CD2-NE2	-5.26	1.32	1.37
1	D	114	HIS	CD2-NE2	-5.18	1.32	1.37
1	A	49	HIS	CG-ND1	-5.15	1.32	1.38
1	E	147	HIS	CG-ND1	-5.13	1.32	1.38
1	E	49	HIS	CD2-NE2	-5.11	1.32	1.37
1	E	60	GLU	CA-CB	-5.06	1.45	1.53

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	42	VAL	N-CA-C	-12.90	101.43	111.62
1	D	49	HIS	CA-CB-CG	-11.46	102.34	113.80
1	C	49	HIS	CA-CB-CG	-10.69	103.11	113.80
1	A	42	VAL	N-CA-C	-10.29	103.49	111.62
1	C	112	ASP	CA-CB-CG	10.25	122.85	112.60
1	E	42	VAL	N-CA-C	-9.81	103.87	111.62
1	E	159	ALA	N-CA-C	9.81	121.97	111.28
1	A	49	HIS	CA-CB-CG	-9.73	104.07	113.80
1	B	42	VAL	N-CA-C	-9.57	104.06	111.62
1	B	39	ARG	CB-CG-CD	-9.15	90.25	111.30
1	E	39	ARG	CB-CG-CD	-9.08	90.42	111.30
1	F	127	ASP	CA-CB-CG	8.91	121.51	112.60
1	D	39	ARG	CB-CG-CD	-8.63	91.46	111.30
1	C	39	ARG	CB-CG-CD	-8.42	91.92	111.30
1	F	39	ARG	CB-CG-CD	-8.28	92.26	111.30
1	A	159	ALA	N-CA-C	8.09	120.82	111.11
1	A	39	ARG	CB-CG-CD	-8.09	92.70	111.30
1	D	159	ALA	N-CA-C	7.50	123.75	111.37
1	F	43	ALA	N-CA-C	7.50	121.50	111.30
1	C	159	ALA	N-CA-C	7.37	120.01	111.02
1	C	35	PHE	CA-CB-CG	-7.32	106.48	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	A	49	HIS	CB-CG-CD2	-7.27	121.75	131.20
1	A	43	ALA	N-CA-C	6.94	120.96	111.17
1	B	114	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	B	142	LYS	CA-CB-CG	-6.84	100.41	114.10
1	C	96	MET	CG-SD-CE	-6.83	85.87	100.90
1	C	114	HIS	CB-CG-CD2	-6.77	122.40	131.20
1	C	43	ALA	N-CA-C	6.76	120.57	111.24
1	D	87	ASP	CA-CB-CG	6.74	119.34	112.60
1	E	174	ASP	CA-CB-CG	6.64	119.24	112.60
1	C	142	LYS	CA-CB-CG	-6.61	100.88	114.10
1	F	114	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	E	36	TYR	N-CA-C	-6.56	104.06	111.14
1	C	132	HIS	CB-CG-CD2	-6.56	122.68	131.20
1	D	114	HIS	CB-CG-CD2	-6.52	122.72	131.20
1	E	142	LYS	CA-CB-CG	-6.49	101.12	114.10
1	F	41	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	107	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	D	132	HIS	CB-CG-CD2	-6.42	122.85	131.20
1	B	49	HIS	CB-CG-CD2	-6.42	122.86	131.20
1	E	132	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	A	147	HIS	CB-CG-CD2	-6.39	122.89	131.20
1	C	147	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	E	43	ALA	N-CA-C	6.25	119.99	111.17
1	F	147	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	E	147	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	D	147	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	D	43	ALA	N-CA-C	6.18	119.77	111.24
1	A	114	HIS	CB-CG-CD2	-6.17	123.18	131.20
1	F	132	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	E	114	HIS	CB-CG-CD2	-6.12	123.24	131.20
1	B	159	ALA	N-CA-C	6.12	121.46	111.37
1	E	38	ASP	CA-CB-CG	6.11	118.71	112.60
1	C	49	HIS	CB-CG-CD2	-6.11	123.26	131.20
1	D	152	GLN	CA-C-O	-6.09	114.09	120.55
1	A	174	ASP	CA-CB-CG	6.08	118.68	112.60
1	B	43	ALA	N-CA-C	6.07	119.77	111.39
1	B	132	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	F	174	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	87	ASP	CA-CB-CG	6.05	118.65	112.60
1	D	174	ASP	CA-CB-CG	6.05	118.65	112.60
1	D	127	ASP	CA-CB-CG	6.04	118.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	142	LYS	CA-CB-CG	-6.03	102.04	114.10
1	B	174	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	124	HIS	CB-CG-CD2	-5.96	123.45	131.20
1	A	7	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	E	7	ASN	OD1-CG-ND2	-5.91	116.69	122.60
1	F	171	LEU	O-C-N	-5.88	114.44	122.33
1	D	7	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	C	174	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	35	PHE	CA-CB-CG	-5.82	107.98	113.80
1	E	35	PHE	CA-CB-CG	-5.82	107.98	113.80
1	C	7	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	C	41	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	132	HIS	CB-CG-CD2	-5.76	123.70	131.20
1	C	147	HIS	CA-C-O	-5.74	114.80	120.82
1	E	124	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	D	107	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	D	118	SER	CA-C-O	-5.67	114.41	120.42
1	C	158	GLN	OE1-CD-NE2	-5.64	116.96	122.60
1	F	36	TYR	N-CA-C	-5.58	105.11	111.14
1	D	142	LYS	CA-CB-CG	-5.57	102.97	114.10
1	B	147	HIS	CB-CG-CD2	-5.55	123.98	131.20
1	A	89	TRP	CG-CD2-CE3	5.54	139.44	133.90
1	A	142	LYS	CA-CB-CG	-5.52	103.06	114.10
1	E	147	HIS	CA-C-O	-5.50	115.05	120.82
1	F	49	HIS	CA-CB-CG	-5.47	108.33	113.80
1	A	51	PHE	CA-CB-CG	-5.46	108.34	113.80
1	C	120	GLN	OE1-CD-NE2	-5.42	117.18	122.60
1	F	159	ALA	N-CA-C	5.42	122.36	110.80
1	B	35	PHE	CA-CB-CG	-5.42	108.39	113.80
1	B	171	LEU	O-C-N	-5.39	115.10	122.33
1	A	87	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	7	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	F	124	HIS	CB-CG-CD2	-5.33	124.27	131.20
1	A	96	MET	CG-SD-CE	-5.33	89.18	100.90
1	B	173	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	B	150	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	37	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	134	LEU	N-CA-C	5.24	116.99	111.28
1	D	35	PHE	CA-CB-CG	-5.23	108.57	113.80
1	D	124	HIS	CB-CG-CD2	-5.23	124.40	131.20
1	A	64	ARG	O-C-N	-5.23	116.68	122.07
1	C	87	ASP	CA-CB-CG	5.22	117.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	HIS	CB-CG-CD2	-5.21	124.43	131.20
1	C	147	HIS	CB-CG-ND1	5.21	130.51	122.70
1	A	96	MET	CB-CA-C	-5.20	102.16	110.79
1	C	107	ASN	OD1-CG-ND2	-5.20	117.41	122.60
1	C	131	SER	N-CA-C	5.19	117.02	111.36
1	F	147	HIS	CB-CG-ND1	5.16	130.44	122.70
1	A	173	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	C	146	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	152	GLN	CA-C-O	-5.14	115.10	120.55
1	D	89	TRP	CE2-CD2-CG	-5.12	101.05	107.20
1	C	37	PHE	CA-CB-CG	-5.12	108.68	113.80
1	E	107	ASN	CA-CB-CG	-5.10	107.50	112.60
1	F	173	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	C	132	HIS	N-CA-C	5.05	120.44	113.97
1	C	173	HIS	CB-CG-CD2	-5.04	124.64	131.20
1	D	158	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	C	114	HIS	CA-CB-CG	-5.01	108.79	113.80

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	1398	0	1377	10	0
1	B	1398	0	1376	15	0
1	C	1398	0	1377	15	0
1	D	1398	0	1377	12	0
1	E	1398	0	1377	14	0
1	F	1398	0	1377	19	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	D	2	0	0	0	0
3	A	51	0	0	1	0
3	B	52	0	0	2	0
3	C	49	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	38	0	0	0	0
3	E	39	0	0	1	0
3	F	43	0	0	0	0
All	All	8665	0	8261	73	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 (73) 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:B:71:GLN:HA	1:C:142:LYS:HD2	1.59	0.84
1:D:142:LYS:HD2	1:F:71:GLN:HA	1.61	0.80
1:A:142:LYS:HD2	1:C:71:GLN:HA	1.64	0.79
1:A:71:GLN:HA	1:B:142:LYS:HD2	1.64	0.78
1:D:71:GLN:HA	1:E:142:LYS:HD2	1.66	0.76
1:C:149:THR:HG21	1:E:41:ASP:HA	1.72	0.71
1:E:71:GLN:HA	1:F:142:LYS:HD2	1.72	0.70
1:B:41:ASP:HA	1:F:149:THR:HG21	1.75	0.68
1:E:150:ASN:ND2	1:E:153:ARG:HH11	1.94	0.66
1:F:150:ASN:ND2	1:F:153:ARG:HH11	1.97	0.62
1:B:150:ASN:ND2	1:B:153:ARG:HH11	1.99	0.60
1:A:150:ASN:ND2	1:A:153:ARG:HH11	2.00	0.60
1:C:150:ASN:ND2	1:C:153:ARG:HH11	2.01	0.59
1:F:56:GLU:HG3	1:F:59:ARG:HH21	1.70	0.57
1:F:170:THR:O	1:F:174:ASP:HB3	2.05	0.57
1:E:20:VAL:HG21	1:E:66:LEU:HD13	1.88	0.56
1:D:170:THR:O	1:D:174:ASP:HB3	2.08	0.54
1:E:170:THR:O	1:E:174:ASP:HB3	2.06	0.54
1:B:170:THR:O	1:B:174:ASP:HB3	2.07	0.54
1:C:154:LEU:HD21	1:E:164:TYR:CD2	2.42	0.54
1:D:19:LEU:HD21	1:D:110:LEU:HD23	1.89	0.53
1:C:170:THR:O	1:C:174:ASP:HB3	2.08	0.53
1:C:135:ASP:OD2	1:C:139:LYS:HE2	2.10	0.52
1:D:150:ASN:ND2	1:D:153:ARG:HH11	2.08	0.51
1:E:149:THR:HG22	3:E:353:HOH:O	2.10	0.51
1:C:20:VAL:HG21	1:C:66:LEU:HD13	1.93	0.50
1:A:170:THR:O	1:A:174:ASP:HB3	2.10	0.50
1:D:117:GLY:HA3	1:D:125:LEU:HD23	1.93	0.49
1:A:24:LEU:HD13	1:A:62:ALA:CB	2.43	0.49
1:A:25:ARG:NH1	1:A:84:PRO:HA	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:19:LEU:HD21	1:F:110:LEU:HD23	1.93	0.49
1:A:20:VAL:HG21	1:A:66:LEU:HD13	1.94	0.48
1:D:20:VAL:HG21	1:D:66:LEU:HD13	1.95	0.48
1:C:117:GLY:HA3	1:C:125:LEU:HD23	1.95	0.48
1:E:150:ASN:ND2	1:E:153:ARG:NH1	2.61	0.48
1:B:20:VAL:HG21	1:B:66:LEU:HD13	1.94	0.48
1:C:56:GLU:HG3	1:C:59:ARG:HH21	1.79	0.47
1:E:24:LEU:HD13	1:E:62:ALA:CB	2.44	0.47
1:F:24:LEU:HD13	1:F:62:ALA:CB	2.45	0.47
1:B:164:TYR:CD2	1:F:154:LEU:HD21	2.51	0.46
1:D:56:GLU:HG3	1:D:59:ARG:HH21	1.81	0.45
1:F:39:ARG:HD3	1:F:41:ASP:OD1	2.17	0.45
1:C:149:THR:HG21	1:E:40:ASP:O	2.16	0.45
1:B:75:ARG:NH2	3:B:562:HOH:O	2.49	0.45
1:B:64:ARG:HH11	1:B:64:ARG:HG3	1.82	0.45
1:B:97:LYS:O	1:B:100:ILE:HG22	2.17	0.44
1:B:164:TYR:O	1:B:168:ARG:HB2	2.17	0.44
1:C:19:LEU:HD21	1:C:110:LEU:HD23	1.99	0.44
1:C:24:LEU:HD13	1:C:62:ALA:CB	2.48	0.44
1:C:67:LYS:O	1:C:71:GLN:HG3	2.17	0.44
1:B:67:LYS:O	1:B:71:GLN:HG3	2.18	0.43
1:F:150:ASN:ND2	1:F:153:ARG:NH1	2.66	0.43
1:F:164:TYR:O	1:F:168:ARG:HB2	2.19	0.43
1:D:24:LEU:HD13	1:D:62:ALA:CB	2.49	0.43
1:D:56:GLU:HG3	1:D:59:ARG:NH2	2.34	0.43
1:E:19:LEU:HD21	1:E:110:LEU:HD23	2.00	0.43
1:B:72:ARG:NH1	3:B:375:HOH:O	2.50	0.43
1:A:75:ARG:NH2	3:A:561:HOH:O	2.51	0.42
1:B:40:ASP:O	1:F:149:THR:HG21	2.19	0.42
1:E:25:ARG:HE	1:E:82:GLN:HB2	1.84	0.42
1:F:147:HIS:O	1:F:151:ILE:HG13	2.19	0.42
1:F:166:PHE:CE2	1:F:171:LEU:HD22	2.55	0.41
1:F:97:LYS:HG3	1:F:148:LEU:HD21	2.02	0.41
1:C:164:TYR:O	1:C:168:ARG:HB2	2.20	0.41
1:F:20:VAL:HG21	1:F:66:LEU:HD13	2.02	0.41
1:B:150:ASN:ND2	1:B:153:ARG:NH1	2.69	0.40
1:A:39:ARG:HD3	1:A:41:ASP:OD1	2.22	0.40
1:D:155:VAL:HA	1:D:159:ALA:HA	2.04	0.40
1:E:164:TYR:O	1:E:168:ARG:HB2	2.21	0.40
1:F:67:LYS:O	1:F:71:GLN:HG3	2.22	0.40
1:D:147:HIS:O	1:D:151:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:PHE:O	1:F:137:GLU:HB2	2.21	0.40
1:A:149:THR:HG22	3:C:351:HOH:O	2.21	0.40

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	172/174 (99%)	168 (98%)	2 (1%)	2 (1%)	10	23
1	B	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
1	C	172/174 (99%)	167 (97%)	5 (3%)	0	100	100
1	D	172/174 (99%)	169 (98%)	2 (1%)	1 (1%)	21	42
1	E	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	21	42
1	F	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	21	42
All	All	1032/1044 (99%)	1007 (98%)	20 (2%)	5 (0%)	24	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	E	3	GLN
1	D	3	GLN
1	F	3	GLN
1	A	157	SER

5.3.2 Protein sidechains [i](#)

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	148/148 (100%)	129 (87%)	19 (13%)	4	8
1	B	148/148 (100%)	130 (88%)	18 (12%)	5	10
1	C	148/148 (100%)	129 (87%)	19 (13%)	4	8
1	D	148/148 (100%)	128 (86%)	20 (14%)	4	7
1	E	148/148 (100%)	132 (89%)	16 (11%)	6	13
1	F	148/148 (100%)	127 (86%)	21 (14%)	3	6
All	All	888/888 (100%)	775 (87%)	113 (13%)	4	9

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	25	ARG
1	A	44	LEU
1	A	56	GLU
1	A	66	LEU
1	A	75	ARG
1	A	81	LEU
1	A	104	LYS
1	A	106	LEU
1	A	111	LEU
1	A	116	LEU
1	A	118	SER
1	A	129	LEU
1	A	134	LEU
1	A	155	VAL
1	A	158	GLN
1	A	168	ARG
1	A	171	LEU
1	A	174	ASP
1	B	18	ARG
1	B	24	LEU
1	B	44	LEU
1	B	66	LEU
1	B	75	ARG
1	B	81	LEU
1	B	104	LYS

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Mol	Chain	Res	Type
1	B	106	LEU
1	B	111	LEU
1	B	116	LEU
1	B	118	SER
1	B	129	LEU
1	B	134	LEU
1	B	155	VAL
1	B	158	GLN
1	B	168	ARG
1	B	171	LEU
1	B	174	ASP
1	C	10	THR
1	C	24	LEU
1	C	44	LEU
1	C	49	HIS
1	C	66	LEU
1	C	75	ARG
1	C	81	LEU
1	C	104	LYS
1	C	106	LEU
1	C	111	LEU
1	C	116	LEU
1	C	118	SER
1	C	129	LEU
1	C	134	LEU
1	C	155	VAL
1	C	158	GLN
1	C	168	ARG
1	C	171	LEU
1	C	174	ASP
1	D	10	THR
1	D	24	LEU
1	D	44	LEU
1	D	49	HIS
1	D	66	LEU
1	D	75	ARG
1	D	81	LEU
1	D	104	LYS
1	D	106	LEU
1	D	111	LEU
1	D	116	LEU
1	D	118	SER

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Mol	Chain	Res	Type
1	D	127	ASP
1	D	129	LEU
1	D	134	LEU
1	D	155	VAL
1	D	158	GLN
1	D	168	ARG
1	D	171	LEU
1	D	174	ASP
1	E	24	LEU
1	E	44	LEU
1	E	56	GLU
1	E	66	LEU
1	E	75	ARG
1	E	81	LEU
1	E	104	LYS
1	E	106	LEU
1	E	111	LEU
1	E	116	LEU
1	E	129	LEU
1	E	134	LEU
1	E	155	VAL
1	E	168	ARG
1	E	171	LEU
1	E	174	ASP
1	F	24	LEU
1	F	25	ARG
1	F	44	LEU
1	F	49	HIS
1	F	56	GLU
1	F	66	LEU
1	F	75	ARG
1	F	81	LEU
1	F	104	LYS
1	F	106	LEU
1	F	111	LEU
1	F	116	LEU
1	F	118	SER
1	F	129	LEU
1	F	134	LEU
1	F	155	VAL
1	F	158	GLN
1	F	161	LEU

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Mol	Chain	Res	Type
1	F	168	ARG
1	F	171	LEU
1	F	174	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	147	HIS
1	A	150	ASN
1	B	49	HIS
1	B	71	GLN
1	B	147	HIS
1	B	150	ASN
1	C	71	GLN
1	C	150	ASN
1	D	120	GLN
1	D	132	HIS
1	D	147	HIS
1	D	150	ASN
1	E	120	GLN
1	E	147	HIS
1	E	150	ASN
1	F	3	GLN
1	F	147	HIS
1	F	150	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.