



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:34 PM UTC

PDB ID : 1HC1 / pdb_00001hc1
Title : CRYSTAL STRUCTURE OF HEXAMERIC HAEMOCYANIN FROM PAN-
ULIRUS INTERRUPTUS REFINED AT 3.2 ANGSTROMS RESOLUTION
Authors : Volbeda, A.; Hol, W.G.J.
Deposited on : 1991-05-15
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **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

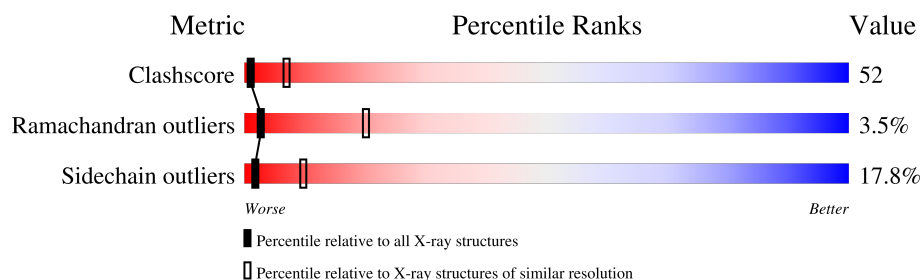
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	657	
1	B	657	
1	C	657	
1	D	657	
1	E	657	
1	F	657	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32166 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 ARTHROPODAN HEMOCYANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	B	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	C	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	D	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	E	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			
1	F	634	Total	C	N	O	S	0	0	0
			5173	3283	892	977	21			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ASP	GLU	conflict	UNP P04254
A	163	PRO	GLN	conflict	UNP P04254
A	458	ASN	LYS	conflict	UNP P04254
A	514	SER	LYS	conflict	UNP P04254
B	32	ASP	GLU	conflict	UNP P04254
B	163	PRO	GLN	conflict	UNP P04254
B	458	ASN	LYS	conflict	UNP P04254
B	514	SER	LYS	conflict	UNP P04254
C	32	ASP	GLU	conflict	UNP P04254
C	163	PRO	GLN	conflict	UNP P04254
C	458	ASN	LYS	conflict	UNP P04254
C	514	SER	LYS	conflict	UNP P04254
D	32	ASP	GLU	conflict	UNP P04254
D	163	PRO	GLN	conflict	UNP P04254
D	458	ASN	LYS	conflict	UNP P04254
D	514	SER	LYS	conflict	UNP P04254
E	32	ASP	GLU	conflict	UNP P04254

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Chain	Residue	Modelled	Actual	Comment	Reference
E	163	PRO	GLN	conflict	UNP P04254
E	458	ASN	LYS	conflict	UNP P04254
E	514	SER	LYS	conflict	UNP P04254
F	32	ASP	GLU	conflict	UNP P04254
F	163	PRO	GLN	conflict	UNP P04254
F	458	ASN	LYS	conflict	UNP P04254
F	514	SER	LYS	conflict	UNP P04254

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cu 2 2	0	0
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0
2	D	2	Total Cu 2 2	0	0
2	E	2	Total Cu 2 2	0	0
2	F	2	Total Cu 2 2	0	0

- Molecule 3 is water.

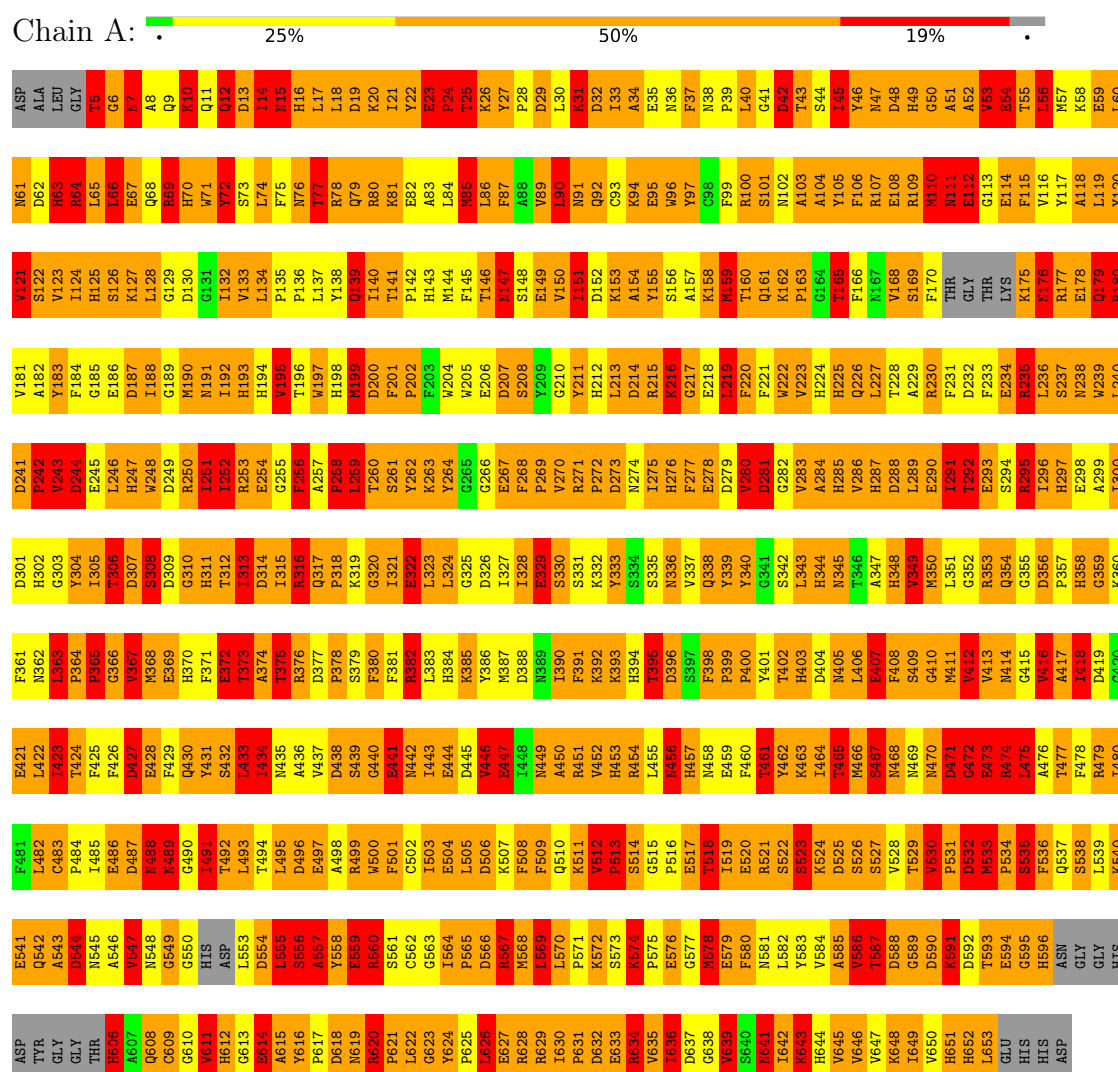
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	186	Total O 186 186	0	0
3	B	186	Total O 186 186	0	0
3	C	186	Total O 186 186	0	0
3	D	186	Total O 186 186	0	0
3	E	186	Total O 186 186	0	0
3	F	186	Total O 186 186	0	0

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.

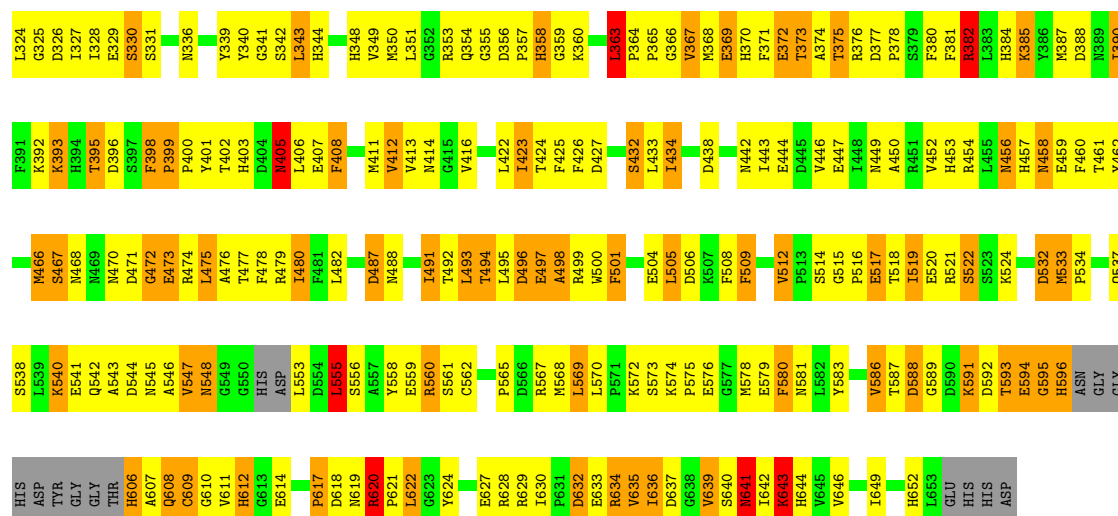
Note EDS was not executed.

• Molecule 1: ARTHROPODAN HEMOCYANIN

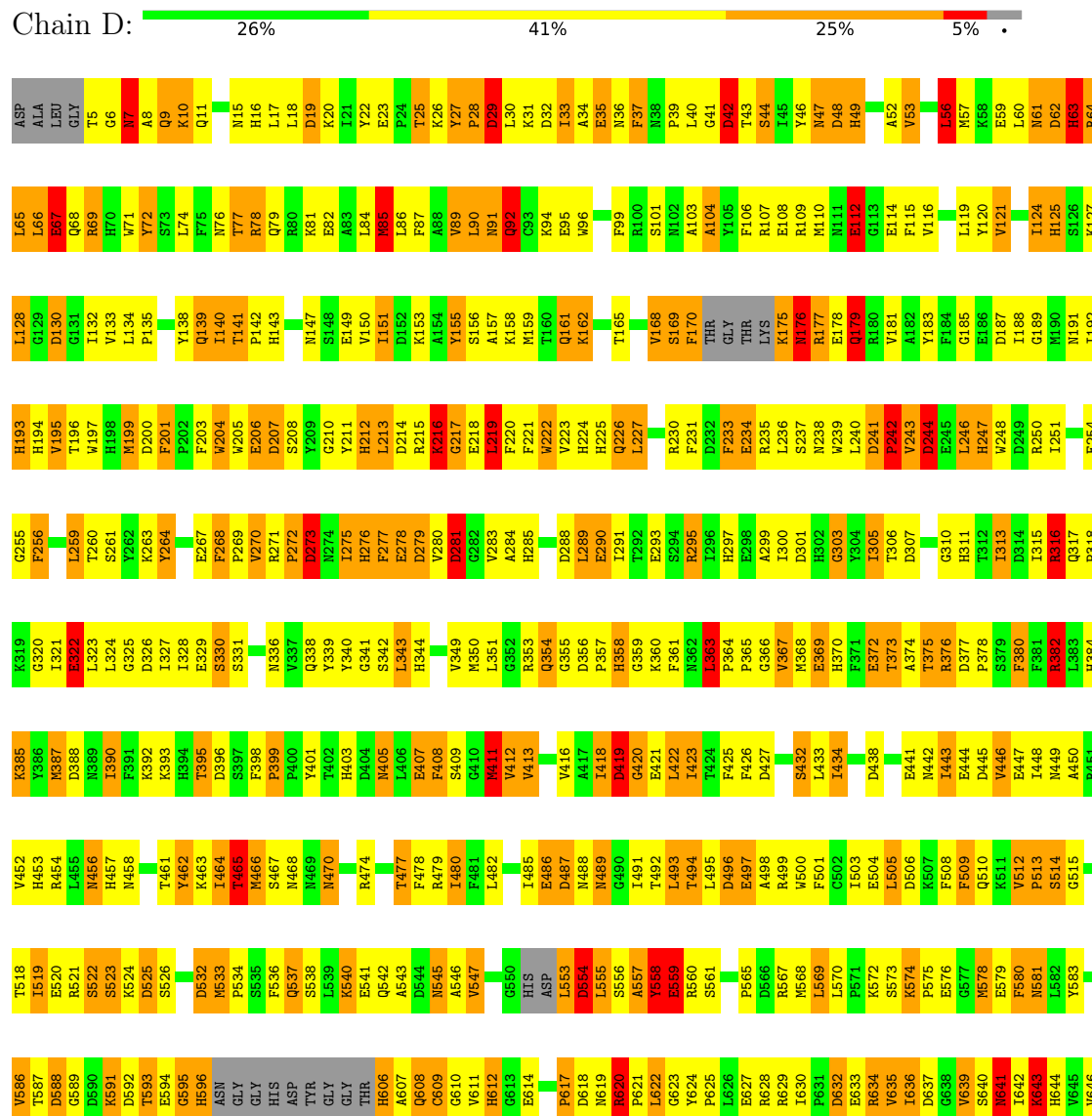


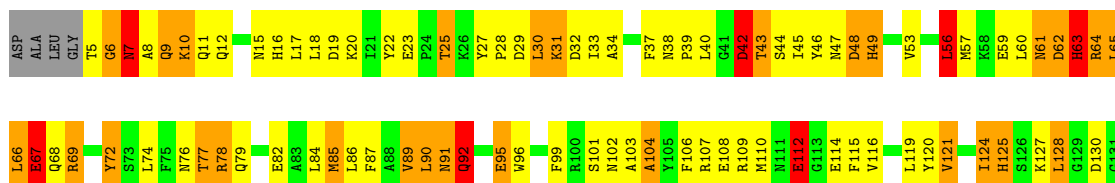
• Molecule 1: ARTHROPODAN HEMOCYANIN





● Molecule 1: ARTHROPODAN HEMOCYANIN





H652	D588	E520	R454	M387	E322	L259	T196
L653	K591	R521	L455	D388	L323	T260	V133
HIS	D592	S522	M456	M389	L324	S261	L134
HIS	E593	S523	H457	I390	G325	Y262	P135
ASP	E594	D532	M458	F391	D326	K263	
	G595	M533	E459	K392	I327	Y264	Y138
	H596	P534	F460	K393	I328		Q139
ASN	GLY	S535	T461	H394	E329		I140
GLY	F536	S536	Y462	T395	S330	F203	T141
GLY	Q537	K463	K463	S397	S331	W204	P142
HIS				F398	R271	E206	H143
ASP				P399	P272	D207	M144
		K540	M466		D273		F145
		E541	S467		D274	G210	
		Q542	M468	T402	R275	Y211	S148
		A543	M469	H403	I276	H212	E149
		D544	N470	D404	H276	L213	L150
		N545	D471	M405	F277	D214	I151
		A546	G472	L406	E278	R215	D152
		F547	E473	E407	D279	K216	K153
		N548	R474	F408	V280	G217	A154
		G549	L475	S409	G281	E218	Y155
		G550	T476	G410	G282	L219	S156
		HIS	T477	M411	V283	F220	A157
		ASP	F478	M412	A284	F221	K158
		L553	R479	M413	H285	W222	M159
		D554	I480	M414		V223	T160
		L555	F481	Q415	D288	H224	Q161
		S556	L482	V416	L289	H225	K162
		A557			E290	Q226	
		Y558	I485	D419	I291	L227	T165
		E559	E486	Q420	T292		
		S561	D487	E421	E293	R230	V168
		G562	N489	L422	S294	F231	S169
		P563	G490	I423	R295	D232	F170
		F564	T491	T424	I296	F233	THR
		P565	T492	F425	H297	E234	GLY
		D566	L493	F426	E298	R235	THR
		R567	T494	D427	A299	L236	LYS
		M568	L495	E428	S237	N237	K175
		L569	D496	D301	I300	N238	N176
		S570	E497	S432	H302	W239	R177
		L570	A498	L433	G303	L240	E178
		P571	R499	I434	Y304	D241	Q179
		K572	W500		I305	P242	R180
		S573	F501	D438	T306	V243	V181
		K574		S439	T373	D244	A182
		P575	E504		D307		Y183
		E576	L505	M442	G310	E245	F184
		G577		I443	H311	L246	G185
		S579	F508	E444	T312	H247	E186
		F580	P509	D445	I313	W248	D187
		N581	V512	V446	D314	D249	I188
		L582	P513	E447	I315	R250	G189
		Y583	S514	I448	R316	I251	M190
		V584		M449	Q317	E252	N191
		A585		A450	R382	R253	I192
		V586	E517	R451	L383	E254	H193
		T587	I519	V452	K384	G255	H194
					K385	F256	V195

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.80Å 193.10Å 122.20Å 90.00° 118.10° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.201 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32166	wwPDB-VP
Average B, all atoms (Å ²)	17.0	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: CU

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	1.82	57/5316 (1.1%)	4.64	1635/7205 (22.7%)
1	B	1.80	69/5316 (1.3%)	4.48	1555/7205 (21.6%)
1	C	0.88	2/5316 (0.0%)	2.19	254/7205 (3.5%)
1	D	0.89	3/5316 (0.1%)	2.20	273/7205 (3.8%)
1	E	0.88	3/5316 (0.1%)	2.17	234/7205 (3.2%)
1	F	0.87	2/5316 (0.0%)	2.18	262/7205 (3.6%)
All	All	1.27	136/31896 (0.4%)	3.18	4213/43230 (9.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

The worst 5 of 136 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	141	THR	CA-CB	8.51	1.63	1.53
1	A	194	HIS	CG-ND1	8.14	1.47	1.38
1	A	216	LYS	C-O	7.95	1.33	1.24
1	A	491	ILE	C-N	-7.90	1.22	1.33
1	A	494	THR	CA-CB	7.67	1.63	1.53

The worst 5 of 4213 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	ARG	NE-CZ-NH2	50.81	164.93	119.20
1	A	64	ARG	CD-NE-CZ	37.85	177.39	124.40
1	B	48	ASP	CA-CB-CG	34.83	147.43	112.60
1	B	17	LEU	O-C-N	26.82	149.69	122.07
1	B	17	LEU	CA-C-O	-26.67	92.81	120.82

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	ARG	Sidechain
1	B	177	ARG	Sidechain
1	B	521	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	5173	0	4888	706	0
1	B	5173	0	4886	674	1
1	C	5173	0	4888	436	3
1	D	5173	0	4888	492	1
1	E	5173	0	4888	447	0
1	F	5173	0	4888	439	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	186	0	0	40	0
3	B	186	0	0	16	0
3	C	186	0	0	12	0
3	D	186	0	0	11	0
3	E	186	0	0	10	0
3	F	186	0	0	9	0
All	All	32166	0	29326	3112	3

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 52.

The worst 5 of 3112 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:GLN:OE1	1:B:443:ILE:HD13	1.28	1.29
1:A:422:LEU:CD2	1:A:570:LEU:HD21	1.66	1.23
1:A:316:ARG:HD3	3:A:829:HOH:O	1.41	1.19
1:A:165:THR:CG2	1:A:449:ASN:HB2	1.73	1.17
1:B:456:ASN:HD22	1:B:457:HIS:N	1.42	1.17

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:OD1	1:C:49:HIS:CD2[2_647]	1.85	0.35
1:C:594:GLU:OE1	1:F:471:ASP:CB[2_657]	2.13	0.07
1:C:474:ARG:NH2	1:D:41:GLY:O[2_656]	2.17	0.03

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	626/657 (95%)	501 (80%)	97 (16%)	28 (4%)	2	15
1	B	626/657 (95%)	506 (81%)	89 (14%)	31 (5%)	1	13
1	C	626/657 (95%)	517 (83%)	95 (15%)	14 (2%)	5	29
1	D	626/657 (95%)	516 (82%)	91 (14%)	19 (3%)	3	23
1	E	626/657 (95%)	512 (82%)	95 (15%)	19 (3%)	3	23
1	F	626/657 (95%)	503 (80%)	102 (16%)	21 (3%)	3	20
All	All	3756/3942 (95%)	3055 (81%)	569 (15%)	132 (4%)	3	20

5 of 132 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	147	ASN
1	A	176	ASN
1	A	441	GLU
1	A	471	ASP

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	564/580 (97%)	416 (74%)	148 (26%)	0	3
1	B	564/580 (97%)	424 (75%)	140 (25%)	1	3
1	C	564/580 (97%)	485 (86%)	79 (14%)	3	17
1	D	564/580 (97%)	475 (84%)	89 (16%)	2	13
1	E	564/580 (97%)	491 (87%)	73 (13%)	4	20
1	F	564/580 (97%)	490 (87%)	74 (13%)	4	19
All	All	3384/3480 (97%)	2781 (82%)	603 (18%)	2	10

5 of 603 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	77	THR
1	F	367	VAL
1	E	216	LYS
1	E	72	TYR
1	E	591	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 174 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	456	ASN
1	E	456	ASN

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Mol	Chain	Res	Type
1	E	11	GLN
1	E	191	ASN
1	F	61	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 12 ligands modelled in this entry, 12 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.