wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:07 PM GMT

PDB ID	:	4BLC
Title	:	THE STRUCTURE OF ORTHORHOMBIC CRYSTALS OF BEEF LIVER CATALASE
Authors	:	Ko, T.P.; Day, J.; Malkin, A.; McPherson, A.
Deposited on	:	1998-09-27
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

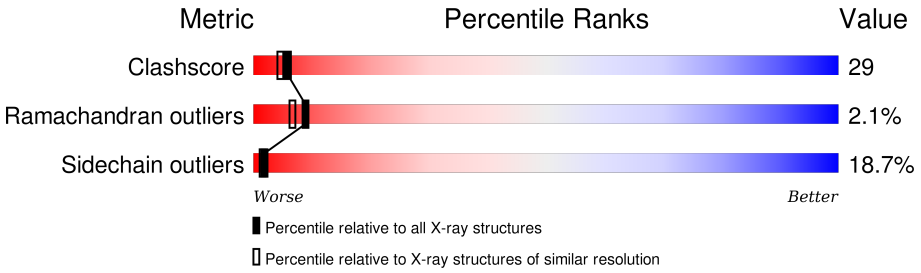
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	506	56% 36% 6% •
1	B	506	38% 45% 15% ••
1	C	506	44% 41% 13% ••
1	D	506	47% 42% 10% •

2 Entry composition

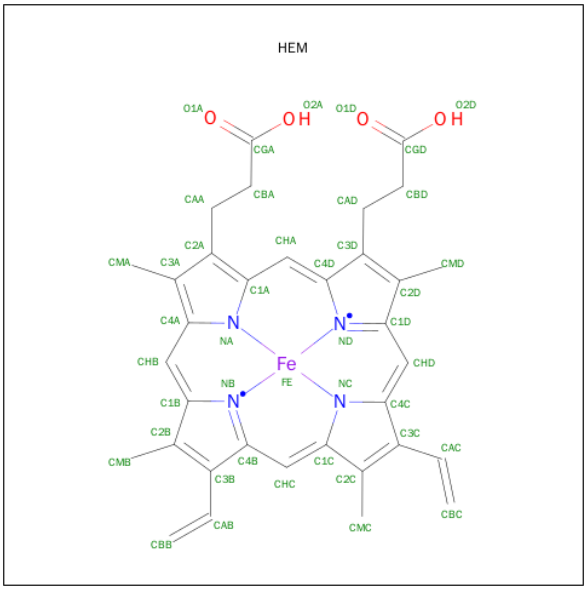
There are 4 unique types of molecules in this entry. The entry contains 16816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	C	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			

- 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		

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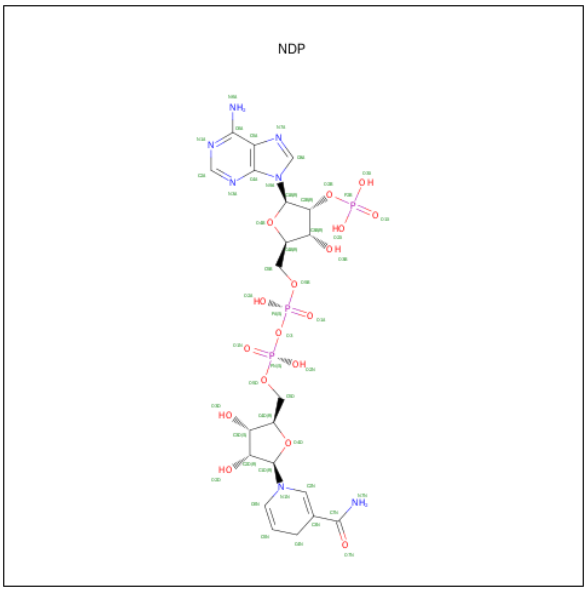
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	89	Total	O	0	0
			89	89		
4	C	83	Total	O	0	0
			83	83		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	93	Total O 93 93	0	0

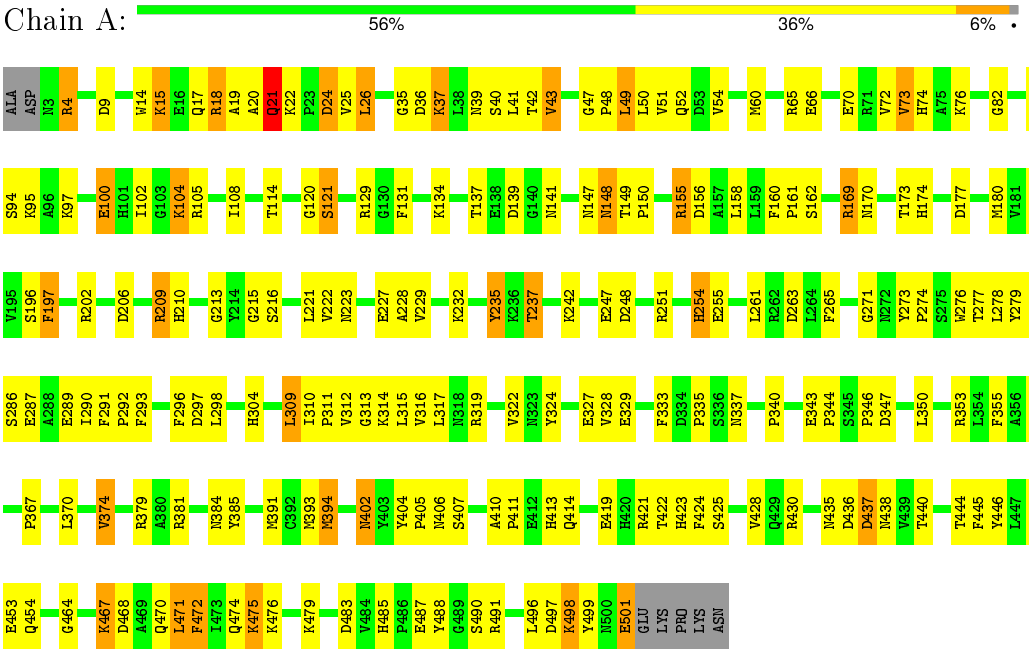
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

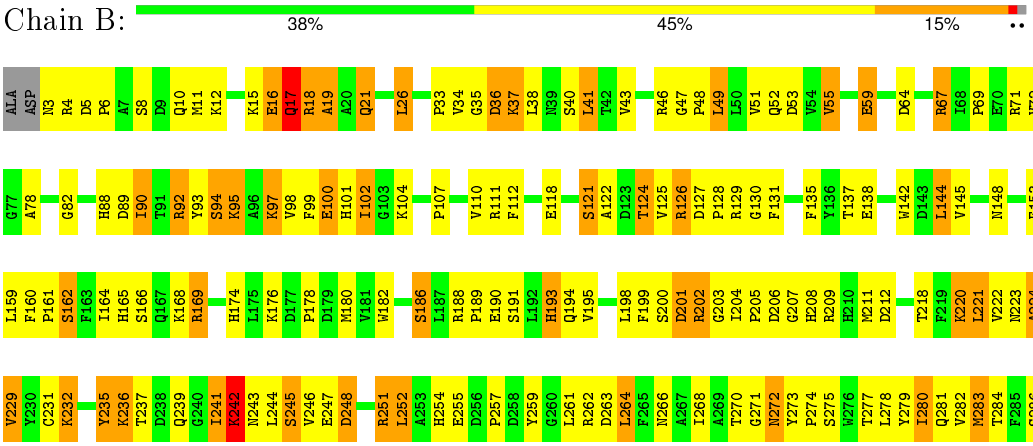
- Molecule 1: PROTEIN (CATALASE)

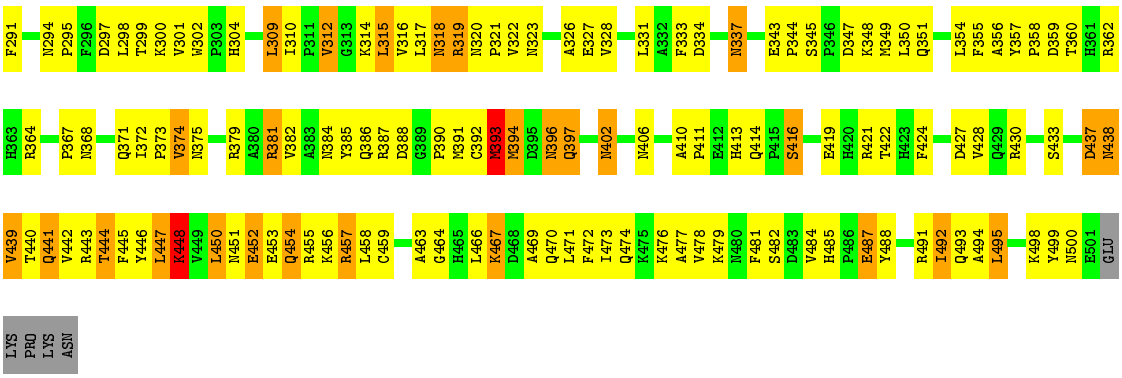
Chain A:



- Molecule 1: PROTEIN (CATALASE)

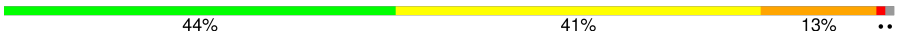
Chain B:

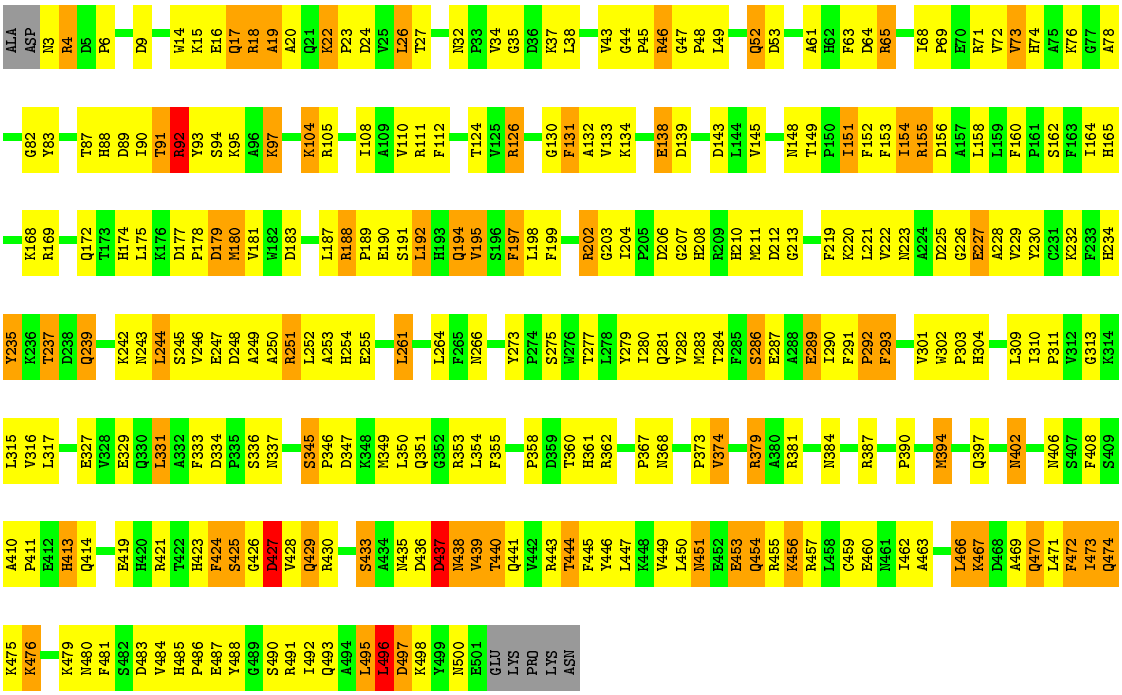




• Molecule 1: PROTEIN (CATALASE)

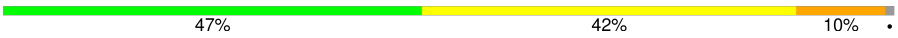
Chain C:

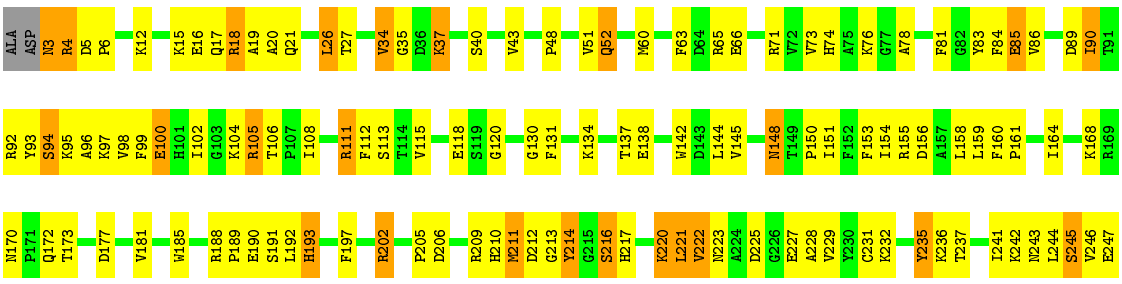


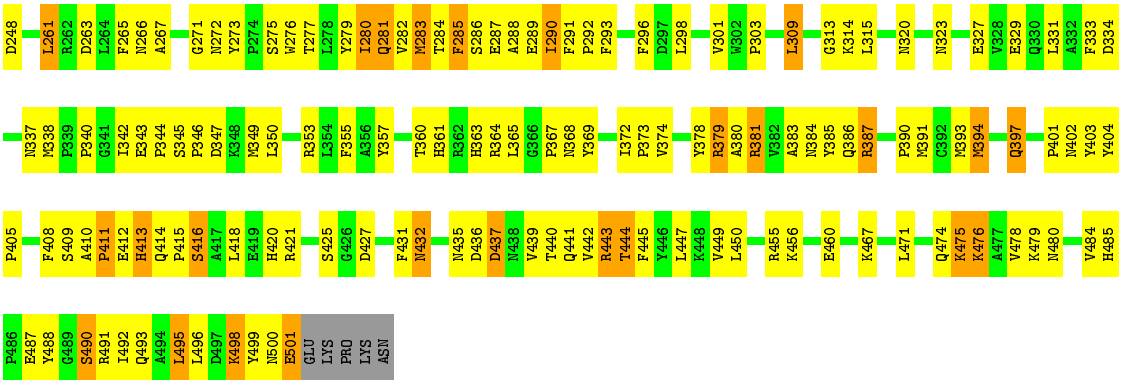


• Molecule 1: PROTEIN (CATALASE)

Chain D:






D248 L261 R262 D263 L264 F265 N266 A267 G271 N272 Y273 P274 S275 W276 T277 L278 Y279 I280 Q281 V282 M283 T284 F285 S286 E287 A288 E289 I290 F291 P292 F293 F296 D297 L298 V301 W302 P303 L309 G313 K314 L315 N320 N323 E327 V328 E329 Q330 L331 A332 F333 D334
N337 M338 P339 P340 G341 I342 E343 P344 S345 P346 D347 K348 M349 L350 R353 L354 F355 A356 Y357 T360 H361 R362 H363 R364 L365 G366 P367 N368 Y369 I372 P373 V374 Y378 R379 A380 R381 V382 A383 N384 Y385 Q386 R387 P390 M391 C392 N393 M394 Q397 P401 N402 Y403 Y404
P405 F408 S409 A410 P411 E412 H413 Q414 P415 S416 A417 L418 E419 H420 R421 S425 G426 D427 F431 N432 N435 D436 D437 N438 V439 T440 Q441 V442 R443 T444 F445 Y446 L447 K448 V449 L450 R455 K456 E460 K467 L471 Q474 K475 K476 A477 V478 K479 N480 V484 H485
P486 E487 Y488 G489 S490 R491 I492 Q493 A494 I495 L496 D497 K498 Y499 N500 E501 GLU LYS PRO LYS ASN

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.80Å 140.60Å 232.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	87.5 (20.00-2.30)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16816	wwPDB-VP
Average B, all atoms (Å^2)	47.0	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: HEM, NDP

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	0.41	0/4137	0.62	0/5619
1	B	0.39	0/4137	0.59	0/5619
1	C	0.39	0/4137	0.60	0/5619
1	D	0.41	0/4137	0.60	0/5619
All	All	0.40	0/16548	0.60	0/22476

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

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	4017	0	3839	171	0
1	B	4017	0	3839	305	0
1	C	4017	0	3839	273	0
1	D	4017	0	3839	253	0
2	A	43	0	30	5	0
2	B	43	0	30	0	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	48	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	4	0
3	C	48	0	26	2	0
3	D	48	0	26	1	0
4	A	119	0	0	8	0
4	B	89	0	0	16	0
4	C	83	0	0	8	0
4	D	93	0	0	10	0
All	All	16816	0	15580	917	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 29.

The worst 5 of 917 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:223:ASN:HD21	1:D:227:GLU:HB3	0.98	1.12
1:A:451:ASN:H	1:A:454:GLN:HE21	1.06	1.01
1:D:223:ASN:ND2	1:D:227:GLU:HB3	1.79	0.98
1:B:169:ARG:HH11	1:B:169:ARG:HG2	1.30	0.95
1:B:457:ARG:HH11	1:B:457:ARG:HB2	1.28	0.95

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	497/506 (98%)	442 (89%)	50 (10%)	5 (1%)	19 21
1	B	497/506 (98%)	423 (85%)	58 (12%)	16 (3%)	5 3
1	C	497/506 (98%)	417 (84%)	65 (13%)	15 (3%)	5 3
1	D	497/506 (98%)	442 (89%)	49 (10%)	6 (1%)	16 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1988/2024 (98%)	1724 (87%)	222 (11%)	42 (2%)	9 7

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	437	ASP
1	B	124	THR
1	B	242	LYS
1	B	394	MET

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	431/437 (99%)	365 (85%)	66 (15%)	3 3
1	B	431/437 (99%)	332 (77%)	99 (23%)	1 1
1	C	431/437 (99%)	349 (81%)	82 (19%)	2 1
1	D	431/437 (99%)	356 (83%)	75 (17%)	2 2
All	All	1724/1748 (99%)	1402 (81%)	322 (19%)	2 1

5 of 322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	447	LEU
1	C	95	LYS
1	D	368	ASN
1	B	454	GLN
1	B	498	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	402	ASN
1	C	52	GLN
1	D	368	ASN
1	B	414	GLN
1	B	441	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

8 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	$\#\|Z\| > 2$
3	NDP	A	1102	-	42,52,52	1.38	6 (14%)	55,80,80	2.04	10 (18%)
2	HEM	A	507	1	30,50,50	2.91	11 (36%)	24,82,82	2.08	8 (33%)
3	NDP	B	1202	-	42,52,52	1.40	4 (9%)	55,80,80	2.44	14 (25%)
2	HEM	B	507	1	30,50,50	2.55	11 (36%)	24,82,82	2.12	7 (29%)
3	NDP	C	1302	-	42,52,52	1.41	5 (11%)	55,80,80	2.26	14 (25%)
2	HEM	C	507	1	30,50,50	2.50	10 (33%)	24,82,82	1.92	6 (25%)
3	NDP	D	1402	-	42,52,52	1.41	6 (14%)	55,80,80	1.91	9 (16%)
2	HEM	D	507	1	30,50,50	2.70	11 (36%)	24,82,82	2.26	8 (33%)

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
3	NDP	A	1102	-	-	0/30/77/77	0/5/5/5
2	HEM	A	507	1	-	0/10/54/54	0/0/8/8
3	NDP	B	1202	-	-	0/30/77/77	0/5/5/5
2	HEM	B	507	1	-	0/10/54/54	0/0/8/8
3	NDP	C	1302	-	-	0/30/77/77	0/5/5/5
2	HEM	C	507	1	-	0/10/54/54	0/0/8/8
3	NDP	D	1402	-	-	0/30/77/77	0/5/5/5
2	HEM	D	507	1	-	0/10/54/54	0/0/8/8

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	507	HEM	C3B-C4B	-6.74	1.45	1.51
2	A	507	HEM	C3B-CAB	-6.66	1.38	1.51
2	A	507	HEM	C3C-CAC	-6.41	1.39	1.51
2	D	507	HEM	C2D-C3D	-6.34	1.35	1.54
2	A	507	HEM	C2D-C3D	-6.18	1.36	1.54

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1202	NDP	N3A-C2A-N1A	-11.77	119.88	128.89
3	C	1302	NDP	N3A-C2A-N1A	-10.39	120.94	128.89
3	D	1402	NDP	N3A-C2A-N1A	-9.19	121.86	128.89
3	A	1102	NDP	N3A-C2A-N1A	-9.10	121.93	128.89
3	B	1202	NDP	C1B-N9A-C4A	-4.65	119.93	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	NDP	3	0
2	A	507	HEM	5	0
3	B	1202	NDP	4	0
3	C	1302	NDP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	507	HEM	4	0
3	D	1402	NDP	1	0
2	D	507	HEM	2	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.