



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 23, 2018 – 09:32 AM EST

PDB ID : 4WJG
Title : Structure of T. brucei haptoglobin-hemoglobin receptor binding to human haptoglobin-hemoglobin
Authors : Støedkilde, K.; Torvund-Jensen, M.; Moestrup, S.K.; Andersen, C.B.F.
Deposited on : 2014-09-30
Resolution : 3.10 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 ⓘ 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-20030736
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-20030736

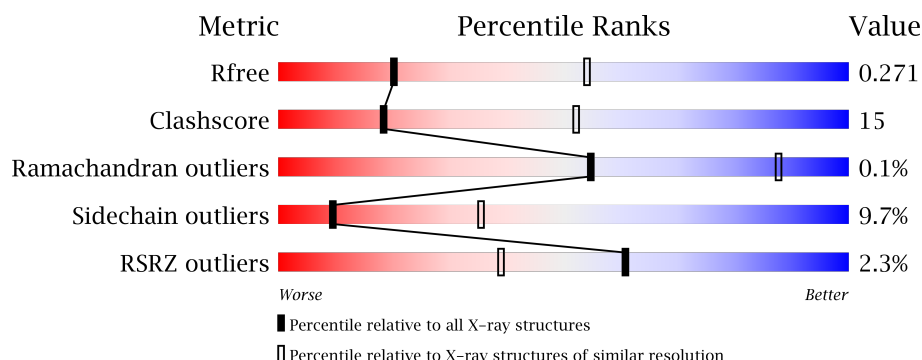
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	141	
1	F	141	
1	K	141	
1	P	141	
1	U	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Z	141	
2	1	146	
2	B	146	
2	G	146	
2	L	146	
2	Q	146	
2	V	146	
3	2	315	
3	C	315	
3	H	315	
3	M	315	
3	R	315	
3	W	315	
4	3	146	
4	D	146	
4	I	146	
4	N	146	
4	S	146	
4	X	146	
5	4	343	
5	E	343	
5	J	343	
5	O	343	
5	T	343	
5	Y	343	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 47792 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	F	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	K	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	P	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	U	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	Z	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	G	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	L	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	Q	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	V	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	1	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is a protein called Haptoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	H	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	M	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	R	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	W	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	2	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			

- Molecule 4 is a protein called Iron-regulated surface determinant protein H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	I	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	N	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	S	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	X	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	3	144	Total	C	N	O	0	0	0
			1183	754	189	240			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	84	GLY	-	expression tag	UNP Q99TD3
D	85	SER	-	expression tag	UNP Q99TD3
I	84	GLY	-	expression tag	UNP Q99TD3
I	85	SER	-	expression tag	UNP Q99TD3
N	84	GLY	-	expression tag	UNP Q99TD3
N	85	SER	-	expression tag	UNP Q99TD3
S	84	GLY	-	expression tag	UNP Q99TD3
S	85	SER	-	expression tag	UNP Q99TD3
X	84	GLY	-	expression tag	UNP Q99TD3
X	85	SER	-	expression tag	UNP Q99TD3
3	84	GLY	-	expression tag	UNP Q99TD3
3	85	SER	-	expression tag	UNP Q99TD3

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 5 | E | 261 | Total
1963 | C
1202 | N
365 | O
393 | S
3 | 0 | 0 | 0 |
| 5 | J | 261 | Total
1963 | C
1202 | N
365 | O
393 | S
3 | 0 | 0 | 0 |
| 5 | O | 261 | Total
1963 | C
1202 | N
365 | O
393 | S
3 | 0 | 0 | 0 |
| 5 | T | 261 | Total
1963 | C
1202 | N
365 | O
393 | S
3 | 0 | 0 | 0 |
| 5 | Y | 261 | Total
1963 | C
1202 | N
365 | O
393 | S
3 | 0 | 0 | 0 |
| 5 | 4 | 261 | Total
1963 | C
1202 | N
365 | O
393 | S
3 | 0 | 0 | 0 |

- # HEM

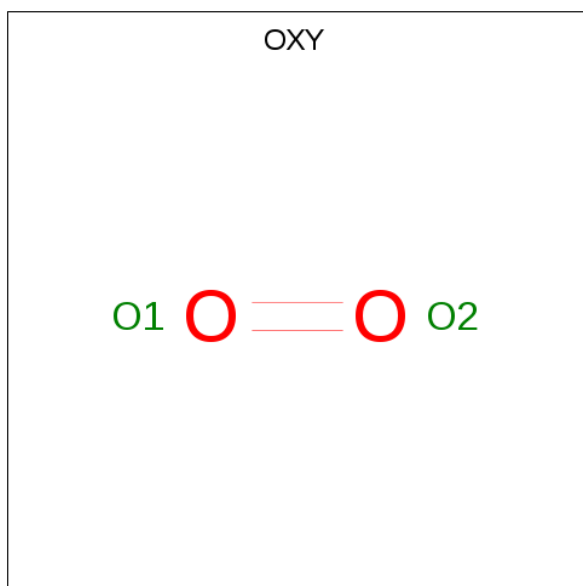
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	Z	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



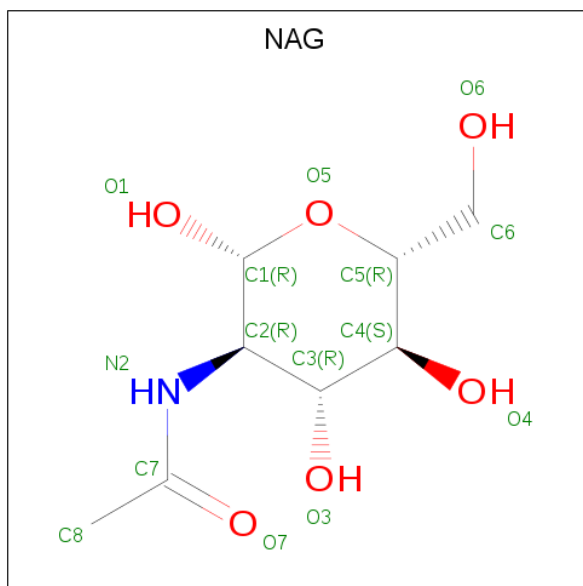
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 2	O 2	0	0
7	B	1	Total 2	O 2	0	0
7	F	1	Total 2	O 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	O	0	0
			2	2		
7	K	1	Total	O	0	0
			2	2		
7	L	1	Total	O	0	0
			2	2		
7	P	1	Total	O	0	0
			2	2		
7	Q	1	Total	O	0	0
			2	2		
7	U	1	Total	O	0	0
			2	2		
7	V	1	Total	O	0	0
			2	2		
7	Z	1	Total	O	0	0
			2	2		
7	1	1	Total	O	0	0
			2	2		

- Molecule 8 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total 14	C 8	N 1	O 5	0	0
8	C	1	Total 14	C 8	N 1	O 5	0	0
8	C	1	Total 14	C 8	N 1	O 5	0	0
8	C	1	Total 14	C 8	N 1	O 5	0	0
8	E	1	Total 14	C 8	N 1	O 5	0	0
8	E	1	Total 14	C 8	N 1	O 5	0	0
8	H	1	Total 14	C 8	N 1	O 5	0	0
8	H	1	Total 14	C 8	N 1	O 5	0	0
8	H	1	Total 14	C 8	N 1	O 5	0	0
8	H	1	Total 14	C 8	N 1	O 5	0	0
8	J	1	Total 14	C 8	N 1	O 5	0	0
8	J	1	Total 14	C 8	N 1	O 5	0	0
8	M	1	Total 14	C 8	N 1	O 5	0	0
8	M	1	Total 14	C 8	N 1	O 5	0	0
8	M	1	Total 14	C 8	N 1	O 5	0	0
8	M	1	Total 14	C 8	N 1	O 5	0	0
8	M	1	Total 14	C 8	N 1	O 5	0	0
8	M	1	Total 14	C 8	N 1	O 5	0	0
8	M	1	Total 14	C 8	N 1	O 5	0	0
8	O	1	Total 14	C 8	N 1	O 5	0	0
8	O	1	Total 14	C 8	N 1	O 5	0	0
8	R	1	Total 14	C 8	N 1	O 5	0	0

Continued on next page...

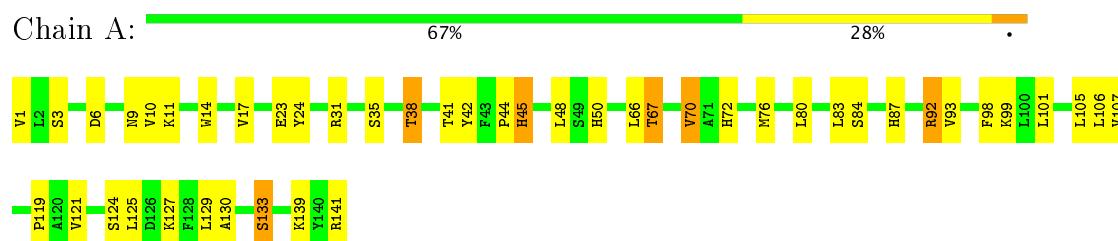
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	T	1	Total	C	N	O	0	0
			14	8	1	5		
8	T	1	Total	C	N	O	0	0
			14	8	1	5		
8	W	1	Total	C	N	O	0	0
			14	8	1	5		
8	W	1	Total	C	N	O	0	0
			14	8	1	5		
8	W	1	Total	C	N	O	0	0
			14	8	1	5		
8	W	1	Total	C	N	O	0	0
			14	8	1	5		
8	Y	1	Total	C	N	O	0	0
			14	8	1	5		
8	Y	1	Total	C	N	O	0	0
			14	8	1	5		
8	2	1	Total	C	N	O	0	0
			14	8	1	5		
8	2	1	Total	C	N	O	0	0
			14	8	1	5		
8	2	1	Total	C	N	O	0	0
			14	8	1	5		
8	2	1	Total	C	N	O	0	0
			14	8	1	5		
8	4	1	Total	C	N	O	0	0
			14	8	1	5		
8	4	1	Total	C	N	O	0	0
			14	8	1	5		

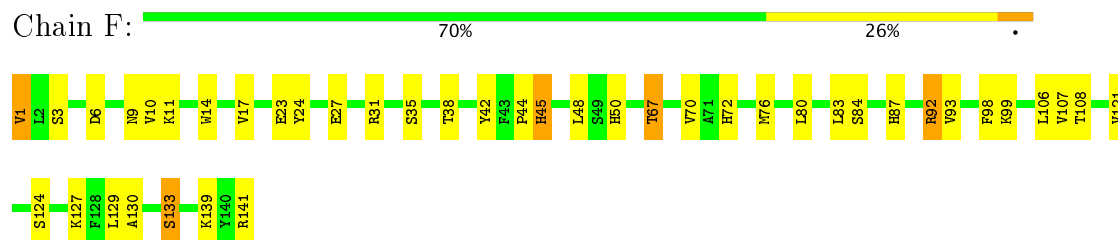
3 Residue-property plots

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.

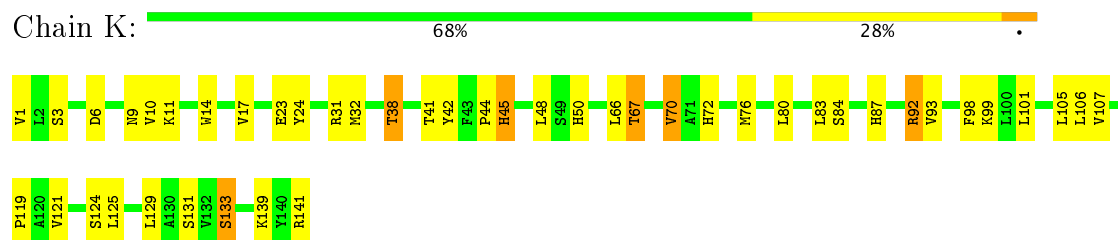
- Molecule 1: Hemoglobin subunit alpha



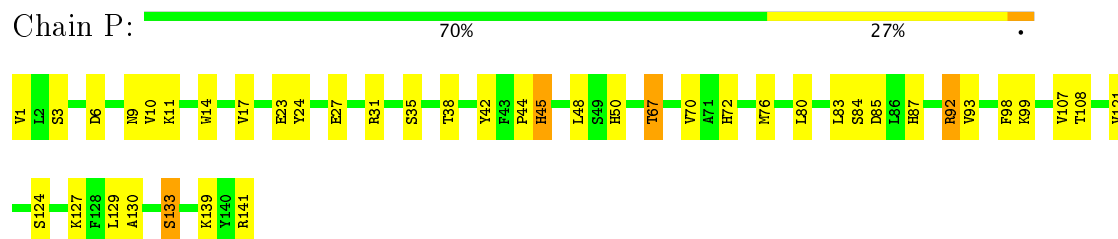
- Molecule 1: Hemoglobin subunit alpha



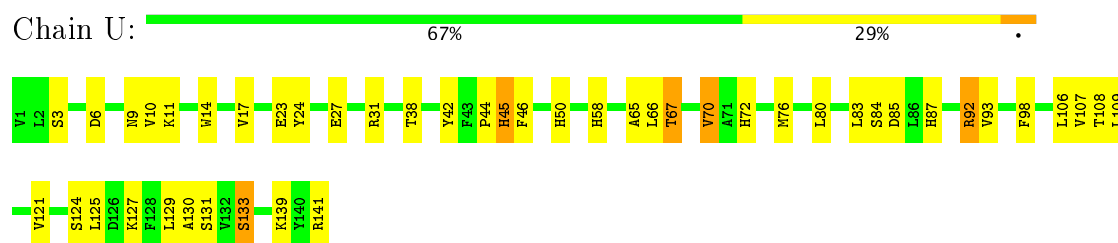
- Molecule 1: Hemoglobin subunit alpha



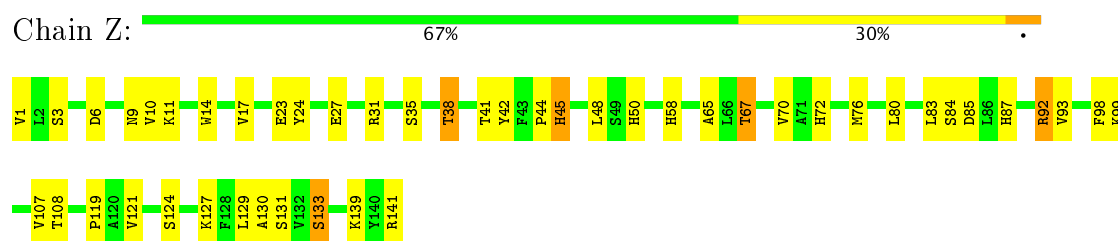
- Molecule 1: Hemoglobin subunit alpha



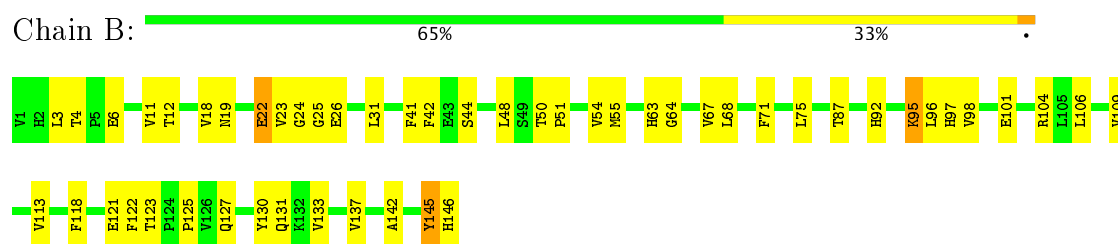
- Molecule 1: Hemoglobin subunit alpha



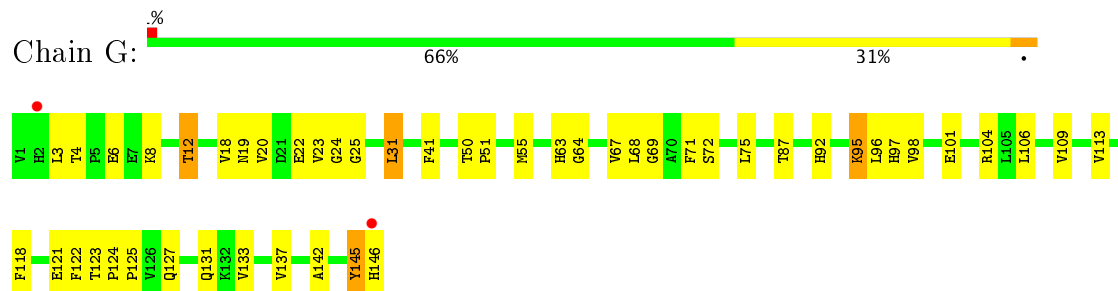
- Molecule 1: Hemoglobin subunit alpha



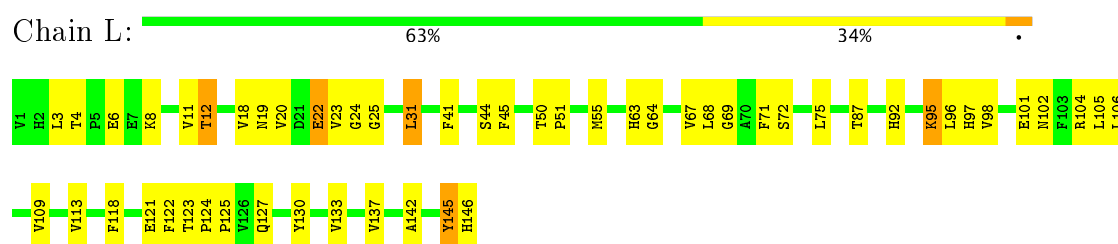
- Molecule 2: Hemoglobin subunit beta



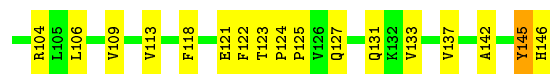
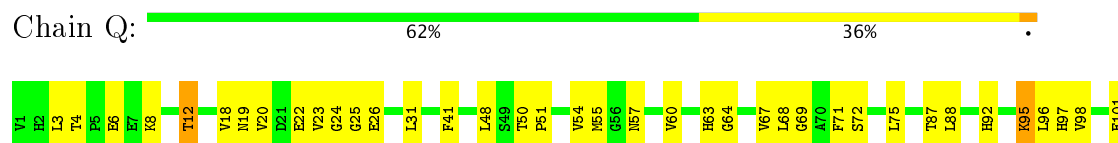
- Molecule 2: Hemoglobin subunit beta



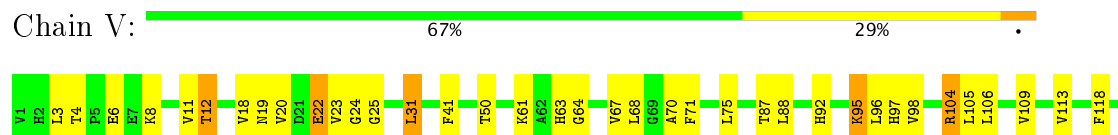
- Molecule 2: Hemoglobin subunit beta



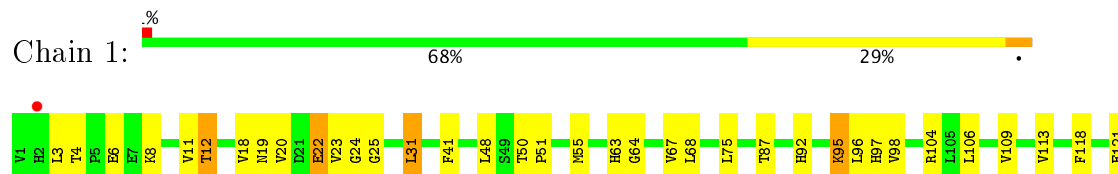
- Molecule 2: Hemoglobin subunit beta



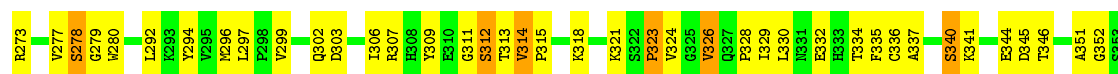
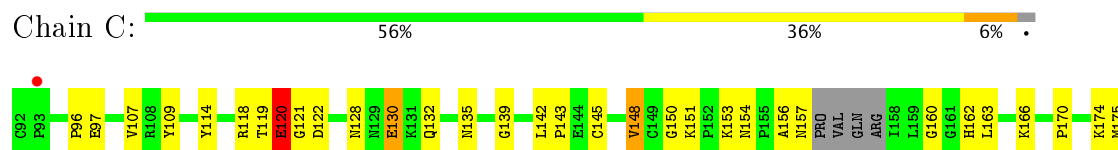
• Molecule 2: Hemoglobin subunit beta



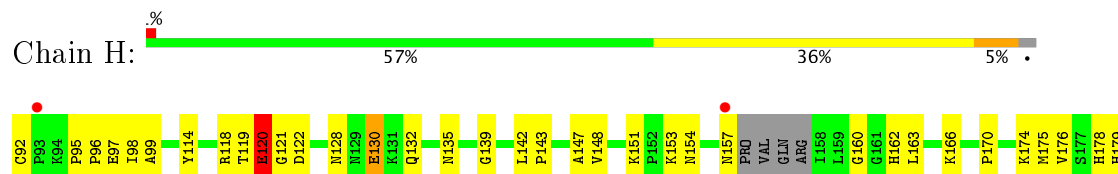
• Molecule 2: Hemoglobin subunit beta



• Molecule 3: Haptoglobin

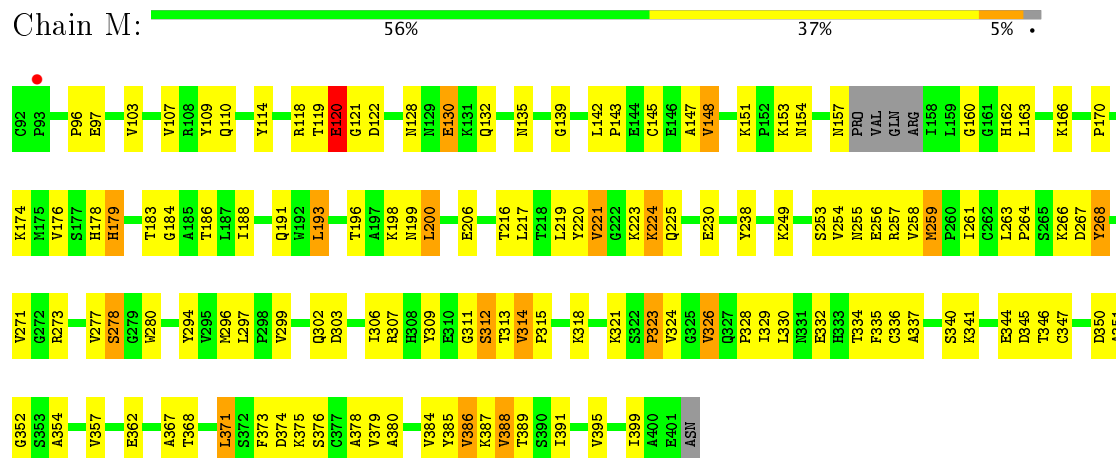


• Molecule 3: Haptoglobin

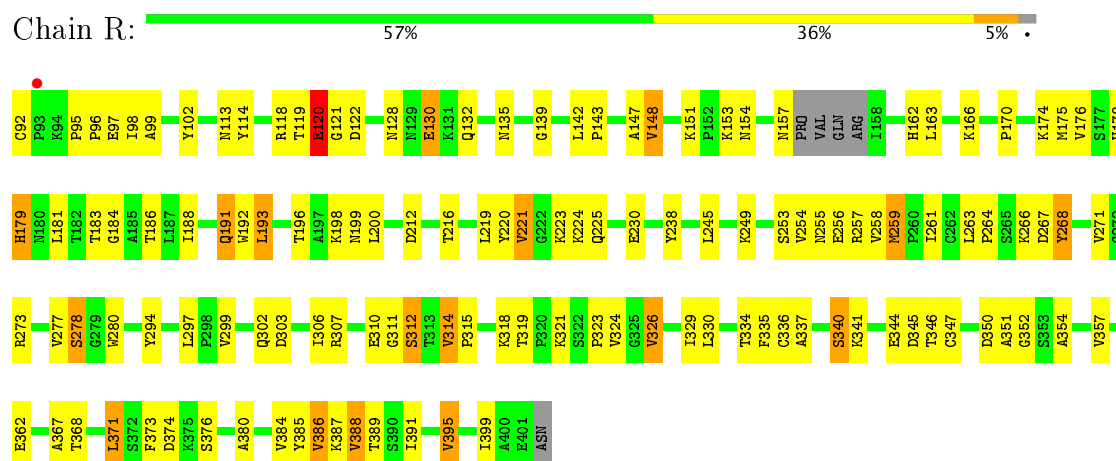




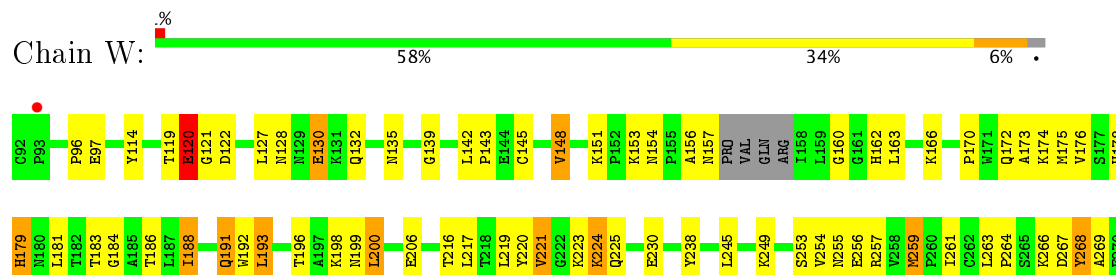
• Molecule 3: Haptoglobin

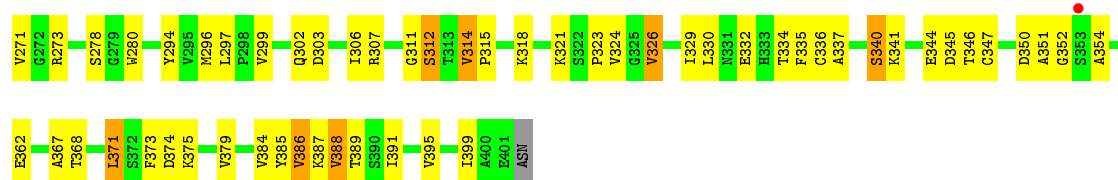


• Molecule 3: Haptoglobin

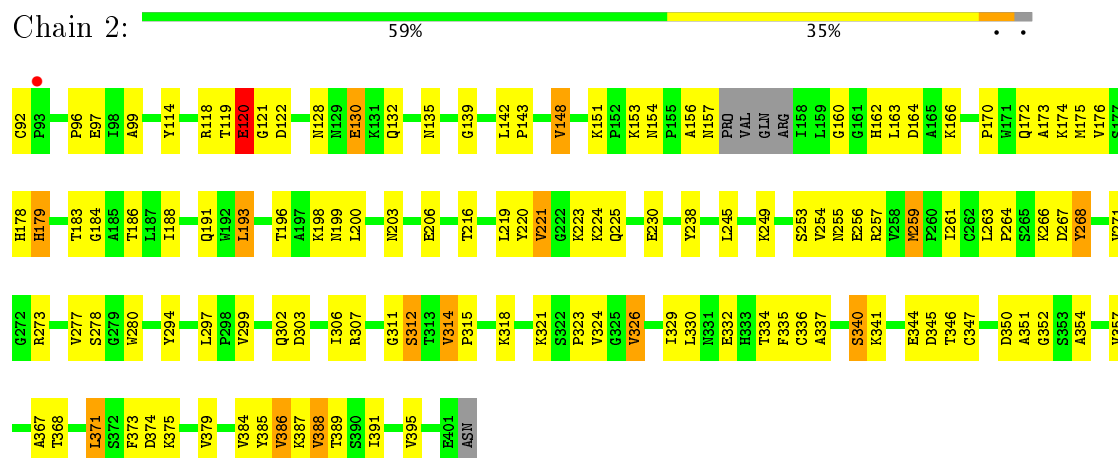


• Molecule 3: Haptoglobin

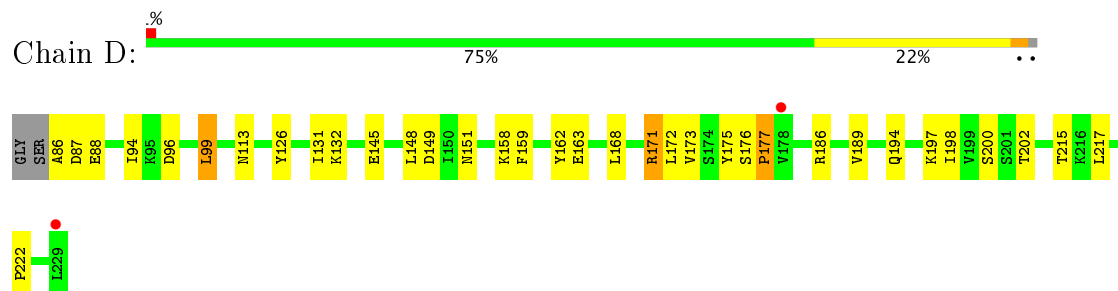




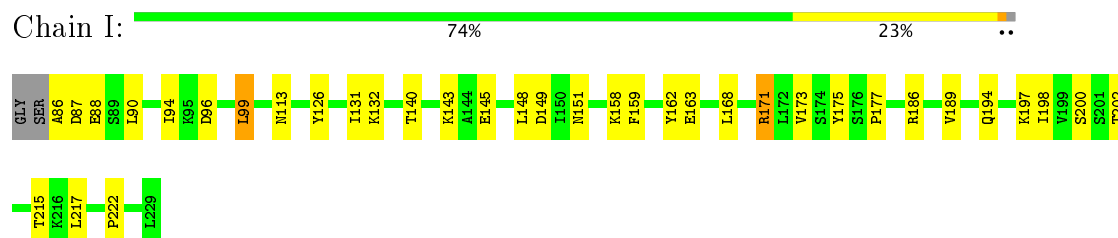
- Molecule 3: Haptoglobin



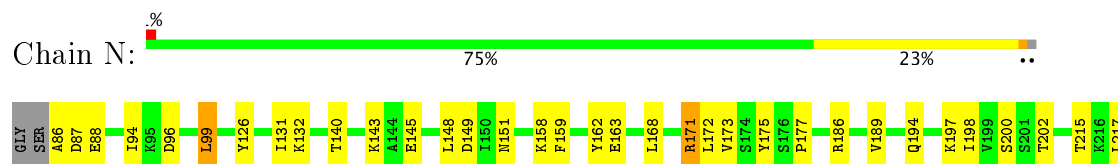
- Molecule 4: Iron-regulated surface determinant protein H



- Molecule 4: Iron-regulated surface determinant protein H



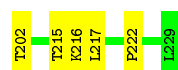
- Molecule 4: Iron-regulated surface determinant protein H





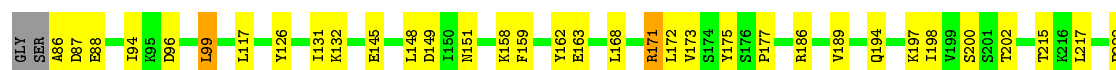
• Molecule 4: Iron-regulated surface determinant protein H

Chain S: 73% 25% ..



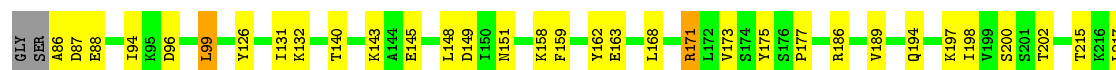
• Molecule 4: Iron-regulated surface determinant protein H

Chain X: 75% 22% ..



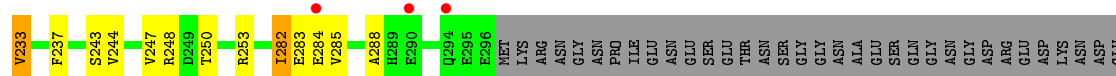
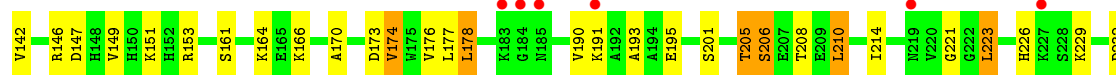
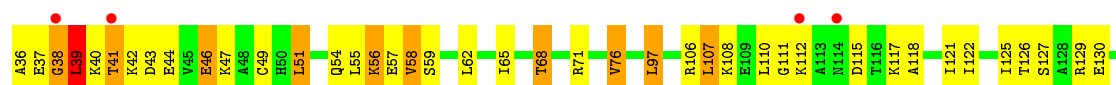
• Molecule 4: Iron-regulated surface determinant protein H

Chain 3: 75% 22% ..

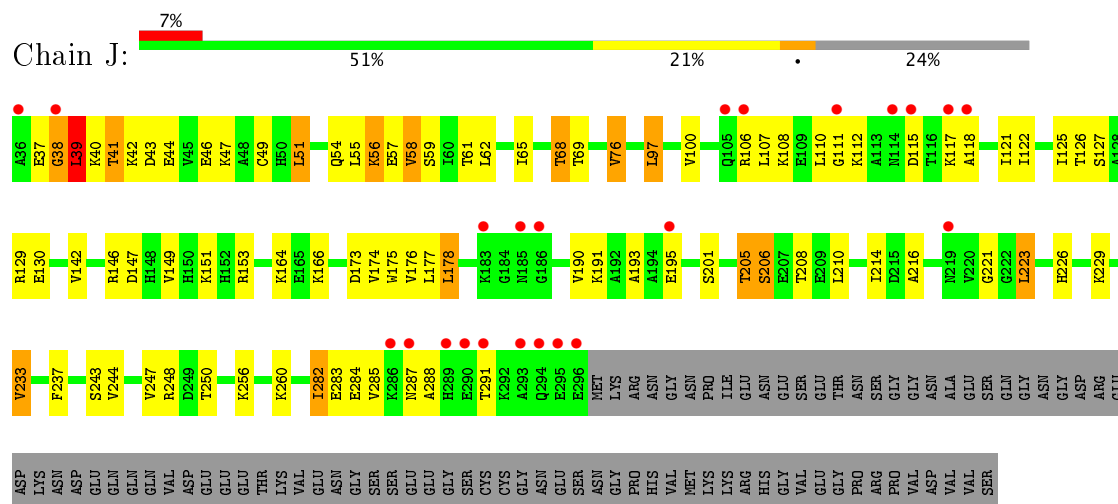


• Molecule 5: Haptoglobin-hemoglobin receptor

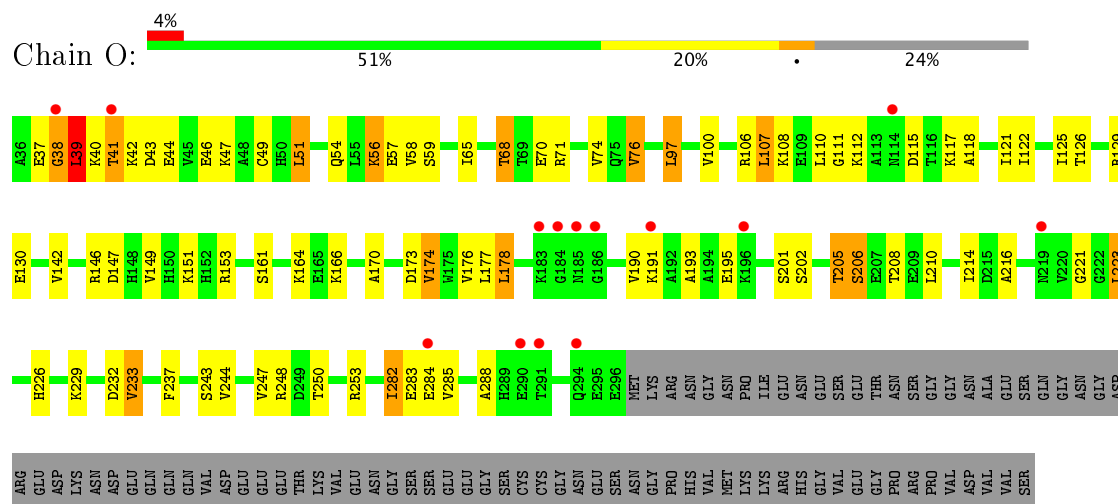
Chain E: 4% 52% 19% 5% 24%



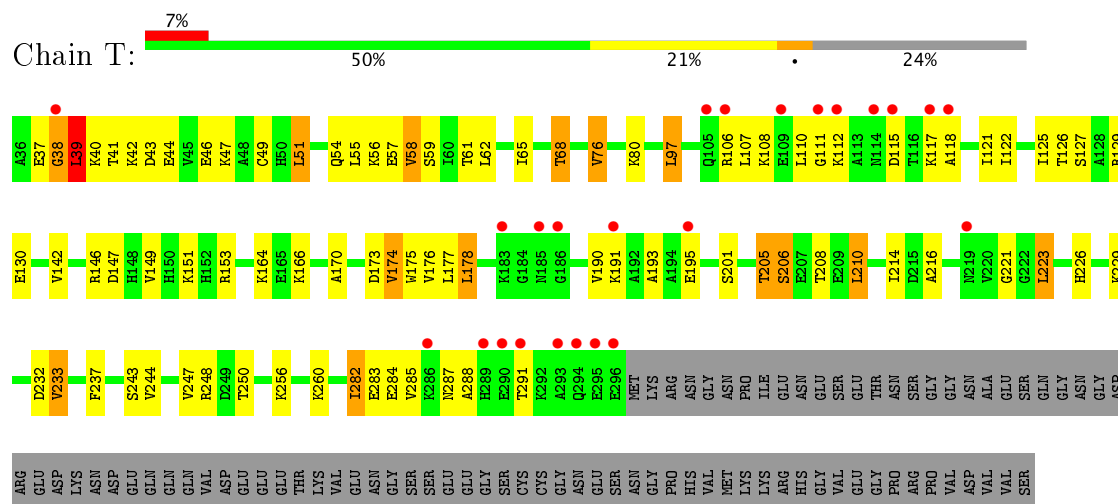
- Molecule 5: Haptoglobin-hemoglobin receptor



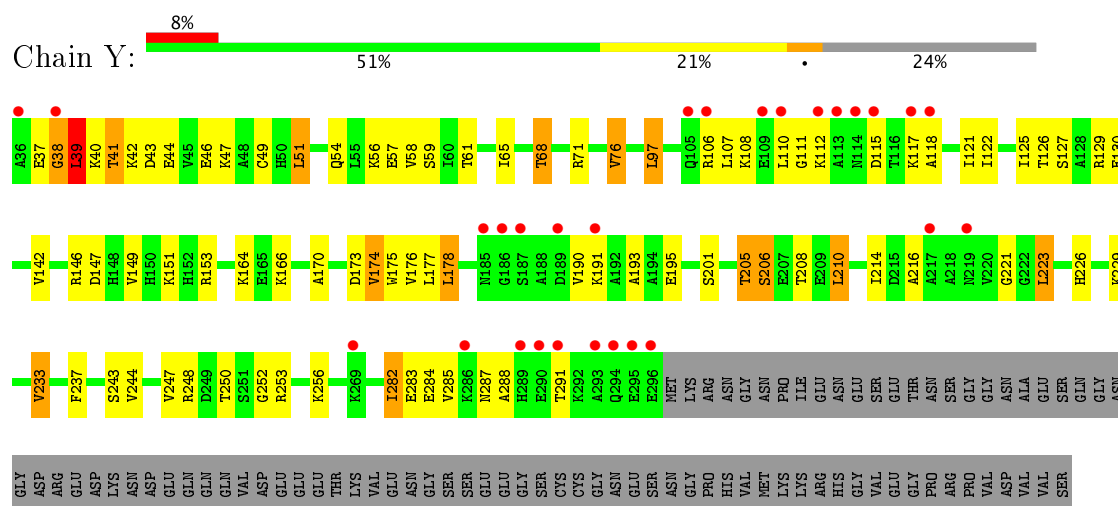
- Molecule 5: Haptoglobin-hemoglobin receptor



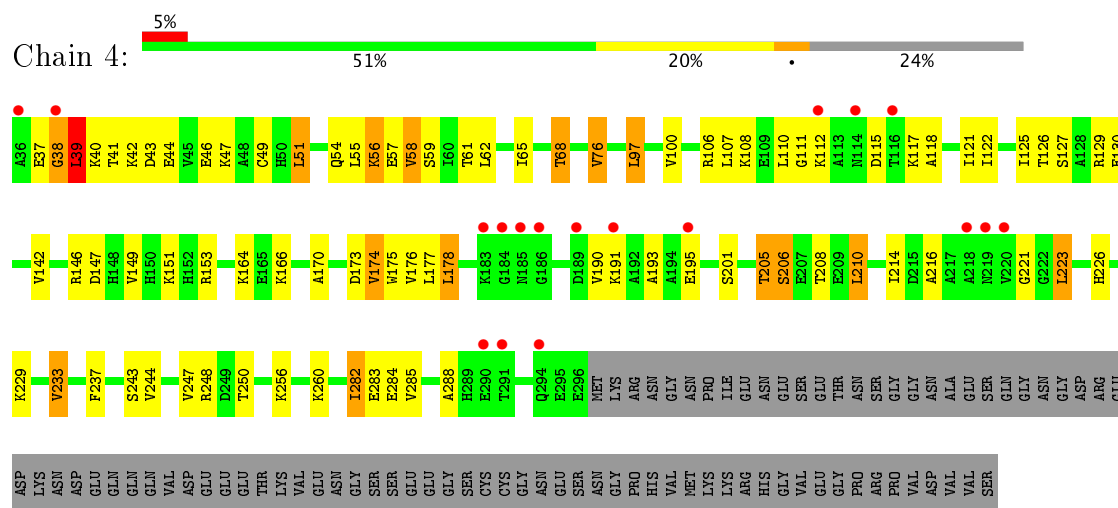
- Molecule 5: Haptoglobin-hemoglobin receptor



- Molecule 5: Haptoglobin-hemoglobin receptor



• Molecule 5: Haptoglobin-hemoglobin receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	143.23Å 140.95Å 267.18Å 90.00° 98.54° 90.00°	Depositor
Resolution (Å)	29.00 – 3.10 28.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.00-3.10) 96.7 (28.98-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, R_{free}	0.255 , 0.271 0.255 , 0.271	Depositor DCC
R_{free} test set	1756 reflections (0.96%)	DCC
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	47792	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.03 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4672e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NAG, OXY

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	0.54	0/1097	0.66	0/1491
1	F	0.52	0/1097	0.69	2/1491 (0.1%)
1	K	0.54	0/1097	0.68	0/1491
1	P	0.51	0/1097	0.64	0/1491
1	U	0.46	0/1097	0.61	0/1491
1	Z	0.47	0/1097	0.61	0/1491
2	1	0.49	0/1153	0.61	0/1566
2	B	0.59	0/1153	0.67	0/1566
2	G	0.57	0/1153	0.65	0/1566
2	L	0.59	0/1153	0.68	0/1566
2	Q	0.56	0/1153	0.65	0/1566
2	V	0.51	0/1153	0.61	0/1566
3	2	0.52	0/2497	0.71	0/3391
3	C	0.64	0/2497	0.77	0/3391
3	H	0.57	0/2497	0.74	0/3391
3	M	0.64	0/2497	0.77	0/3391
3	R	0.57	0/2497	0.74	0/3391
3	W	0.49	0/2497	0.71	0/3391
4	3	0.44	0/1212	0.62	0/1647
4	D	0.51	0/1212	0.66	0/1647
4	I	0.49	0/1212	0.65	0/1647
4	N	0.52	0/1212	0.66	0/1647
4	S	0.49	0/1212	0.65	0/1647
4	X	0.43	0/1212	0.63	0/1647
5	4	0.41	0/1981	0.62	1/2666 (0.0%)
5	E	0.45	0/1981	0.63	1/2666 (0.0%)
5	J	0.42	0/1981	0.62	1/2666 (0.0%)
5	O	0.48	0/1981	0.64	1/2666 (0.0%)
5	T	0.42	0/1981	0.62	1/2666 (0.0%)
5	Y	0.39	0/1981	0.61	1/2666 (0.0%)
All	All	0.52	0/47640	0.67	8/64566 (0.0%)

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
3	2	0	3
3	C	0	4
3	H	0	3
3	M	0	4
3	R	0	3
3	W	0	3
4	3	0	1
4	D	0	1
4	I	0	1
4	N	0	1
4	S	0	1
4	X	0	1
5	4	0	1
5	E	0	1
5	J	0	1
5	O	0	1
5	T	0	1
5	Y	0	1
All	All	0	32

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1	VAL	CG1-CB-CG2	6.10	120.66	110.90
1	F	1	VAL	CB-CA-C	-5.41	101.12	111.40
5	E	223	LEU	CA-CB-CG	5.25	127.38	115.30
5	T	223	LEU	CA-CB-CG	5.12	127.07	115.30
5	4	223	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	120	GLU	Peptide
3	C	311	GLY	Peptide
3	C	312	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	378	ALA	Peptide
4	D	177	PRO	Peptide

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	1069	0	1073	30	0
1	F	1069	0	1073	27	0
1	K	1069	0	1073	30	0
1	P	1069	0	1073	24	0
1	U	1069	0	1073	33	0
1	Z	1069	0	1073	31	0
2	1	1123	0	1118	32	0
2	B	1123	0	1118	37	0
2	G	1123	0	1118	30	0
2	L	1123	0	1118	39	0
2	Q	1123	0	1118	34	0
2	V	1123	0	1118	33	0
3	2	2437	0	2388	96	0
3	C	2437	0	2387	104	0
3	H	2437	0	2388	100	0
3	M	2437	0	2387	104	0
3	R	2437	0	2387	103	0
3	W	2437	0	2388	95	0
4	3	1183	0	1132	16	0
4	D	1183	0	1132	19	0
4	I	1183	0	1132	17	0
4	N	1183	0	1132	18	0
4	S	1183	0	1132	17	0
4	X	1183	0	1132	17	0
5	4	1963	0	1978	57	0
5	E	1963	0	1978	65	0
5	J	1963	0	1978	60	0
5	O	1963	0	1978	58	0
5	T	1963	0	1978	58	0
5	Y	1963	0	1978	62	0
6	1	43	0	30	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	43	0	30	1	0
6	B	43	0	30	6	0
6	F	43	0	30	2	0
6	G	43	0	30	3	0
6	K	43	0	30	1	0
6	L	43	0	30	6	0
6	P	43	0	30	2	0
6	Q	43	0	30	4	0
6	U	43	0	30	4	0
6	V	43	0	30	3	0
6	Z	43	0	30	2	0
7	1	2	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	F	2	0	0	0	0
7	G	2	0	0	0	0
7	K	2	0	0	0	0
7	L	2	0	0	0	0
7	P	2	0	0	0	0
7	Q	2	0	0	0	0
7	U	2	0	0	1	0
7	V	2	0	0	1	0
7	Z	2	0	0	1	0
8	2	70	0	63	3	0
8	4	28	0	26	2	0
8	C	84	0	76	3	0
8	E	28	0	26	1	0
8	H	56	0	51	3	0
8	J	28	0	26	2	0
8	M	84	0	76	4	0
8	O	28	0	26	1	0
8	R	84	0	76	3	0
8	T	28	0	26	1	0
8	W	56	0	51	2	0
8	Y	28	0	26	1	0
All	All	47792	0	47040	1408	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 15.

The worst 5 of 1408 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)
5:E:43:ASP:OD2	5:E:47:LYS:HE2	1.30	1.29
5:E:43:ASP:OD2	5:E:47:LYS:CE	2.15	0.94
3:2:183:THR:HB	3:2:199:ASN:HD22	1.36	0.89
3:M:183:THR:HB	3:M:199:ASN:HD22	1.35	0.89
5:O:57:GLU:HG3	5:O:201:SER:HB3	1.55	0.88

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	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
1	F	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	K	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	P	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
1	U	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
1	Z	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
2	1	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	G	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	L	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	Q	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	V	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
3	2	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
3	C	306/315 (97%)	285 (93%)	21 (7%)	0	100	100
3	H	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
3	M	306/315 (97%)	282 (92%)	24 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
3	W	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
4	3	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
4	D	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	I	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
4	N	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	S	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	X	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
5	4	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	38	75
5	E	259/343 (76%)	231 (89%)	27 (10%)	1 (0%)	38	75
5	J	259/343 (76%)	234 (90%)	24 (9%)	1 (0%)	38	75
5	O	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	38	75
5	T	259/343 (76%)	233 (90%)	25 (10%)	1 (0%)	38	75
5	Y	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	38	75
All	All	5940/6546 (91%)	5522 (93%)	412 (7%)	6 (0%)	55	88

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	39	LEU
5	J	39	LEU
5	O	39	LEU
5	T	39	LEU
5	Y	39	LEU

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	113/113 (100%)	100 (88%)	13 (12%)	6	27
1	F	113/113 (100%)	100 (88%)	13 (12%)	6	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	113/113 (100%)	100 (88%)	13 (12%)	6	27
1	P	113/113 (100%)	100 (88%)	13 (12%)	6	27
1	U	113/113 (100%)	101 (89%)	12 (11%)	8	30
1	Z	113/113 (100%)	100 (88%)	13 (12%)	6	27
2	1	118/118 (100%)	106 (90%)	12 (10%)	8	32
2	B	118/118 (100%)	107 (91%)	11 (9%)	10	38
2	G	118/118 (100%)	107 (91%)	11 (9%)	10	38
2	L	118/118 (100%)	106 (90%)	12 (10%)	8	32
2	Q	118/118 (100%)	108 (92%)	10 (8%)	12	44
2	V	118/118 (100%)	106 (90%)	12 (10%)	8	32
3	2	266/271 (98%)	238 (90%)	28 (10%)	8	31
3	C	266/271 (98%)	237 (89%)	29 (11%)	7	30
3	H	266/271 (98%)	237 (89%)	29 (11%)	7	30
3	M	266/271 (98%)	235 (88%)	31 (12%)	6	26
3	R	266/271 (98%)	235 (88%)	31 (12%)	6	26
3	W	266/271 (98%)	236 (89%)	30 (11%)	7	28
4	3	133/134 (99%)	129 (97%)	4 (3%)	46	79
4	D	133/134 (99%)	129 (97%)	4 (3%)	46	79
4	I	133/134 (99%)	127 (96%)	6 (4%)	32	68
4	N	133/134 (99%)	129 (97%)	4 (3%)	46	79
4	S	133/134 (99%)	128 (96%)	5 (4%)	38	74
4	X	133/134 (99%)	128 (96%)	5 (4%)	38	74
5	4	202/272 (74%)	180 (89%)	22 (11%)	7	30
5	E	202/272 (74%)	178 (88%)	24 (12%)	6	25
5	J	202/272 (74%)	180 (89%)	22 (11%)	7	30
5	O	202/272 (74%)	179 (89%)	23 (11%)	7	27
5	T	202/272 (74%)	180 (89%)	22 (11%)	7	30
5	Y	202/272 (74%)	180 (89%)	22 (11%)	7	30
All	All	4992/5448 (92%)	4506 (90%)	486 (10%)	9	35

5 of 486 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	N	171	ARG
3	R	148	VAL
3	2	278	SER
5	O	56	LYS
1	P	23	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
3	M	327	GLN
2	Q	131	GLN
3	2	100	HIS
4	N	113	ASN
5	O	54	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

67 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
6	HEM	1	201	2,7	28,50,50	2.58	8 (28%)	17,82,82	1.97	6 (35%)
7	OXY	1	202	6	1,1,1	0.31	0	0,0,0	0.00	-
8	NAG	2	1001	3	14,14,15	0.25	0	15,19,21	0.60	0
8	NAG	2	1002	8,3	14,14,15	0.35	0	15,19,21	1.37	1 (6%)
8	NAG	2	1003	8	14,14,15	0.80	1 (7%)	15,19,21	0.93	1 (6%)
8	NAG	2	1004	8,3	14,14,15	0.82	1 (7%)	15,19,21	1.87	5 (33%)
8	NAG	2	1005	8	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
8	NAG	4	1001	5	14,14,15	0.19	0	15,19,21	0.56	0
8	NAG	4	1002	5	14,14,15	0.82	1 (7%)	15,19,21	0.73	0
6	HEM	A	201	1,7	28,50,50	2.06	5 (17%)	17,82,82	1.82	5 (29%)
7	OXY	A	202	6	1,1,1	0.26	0	0,0,0	0.00	-
6	HEM	B	201	2,7	28,50,50	2.39	7 (25%)	17,82,82	2.33	5 (29%)
7	OXY	B	202	6	1,1,1	0.27	0	0,0,0	0.00	-
8	NAG	C	1001	3	14,14,15	0.44	0	15,19,21	0.63	0
8	NAG	C	1002	8,3	14,14,15	1.11	1 (7%)	15,19,21	1.83	2 (13%)
8	NAG	C	1003	8	14,14,15	1.13	2 (14%)	15,19,21	1.28	1 (6%)
8	NAG	C	1004	3	14,14,15	1.08	1 (7%)	15,19,21	1.06	1 (6%)
8	NAG	C	1005	8,3	14,14,15	0.60	0	15,19,21	2.13	5 (33%)
8	NAG	C	1006	8	14,14,15	0.23	0	15,19,21	0.67	0
8	NAG	E	1001	5	14,14,15	0.32	0	15,19,21	0.58	0
8	NAG	E	1002	5	14,14,15	0.73	1 (7%)	15,19,21	1.21	1 (6%)
6	HEM	F	201	1,7	28,50,50	2.19	7 (25%)	17,82,82	1.92	4 (23%)
7	OXY	F	202	6	1,1,1	0.24	0	0,0,0	0.00	-
6	HEM	G	201	2,7	28,50,50	2.50	8 (28%)	17,82,82	2.00	7 (41%)
7	OXY	G	202	6	1,1,1	0.27	0	0,0,0	0.00	-
8	NAG	H	1001	3	14,14,15	0.67	1 (7%)	15,19,21	0.70	0
8	NAG	H	1002	3	14,14,15	0.60	0	15,19,21	0.68	0
8	NAG	H	1003	8,3	14,14,15	0.99	1 (7%)	15,19,21	2.11	5 (33%)
8	NAG	H	1004	8	14,14,15	0.57	0	15,19,21	0.88	1 (6%)
8	NAG	J	1001	5	14,14,15	0.38	0	15,19,21	0.58	0
8	NAG	J	1002	5	14,14,15	0.67	1 (7%)	15,19,21	0.53	0
6	HEM	K	201	1,7	28,50,50	2.18	7 (25%)	17,82,82	2.38	7 (41%)
7	OXY	K	202	6	1,1,1	0.24	0	0,0,0	0.00	-
6	HEM	L	201	2,7	28,50,50	2.42	9 (32%)	17,82,82	2.53	8 (47%)
7	OXY	L	202	6	1,1,1	0.29	0	0,0,0	0.00	-
8	NAG	M	1001	3	14,14,15	0.92	1 (7%)	15,19,21	0.88	1 (6%)
8	NAG	M	1002	8,3	14,14,15	0.50	0	15,19,21	2.08	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	NAG	M	1003	8	14,14,15	1.19	2 (14%)	15,19,21	1.21	1 (6%)
8	NAG	M	1004	3	14,14,15	1.15	1 (7%)	15,19,21	1.00	1 (6%)
8	NAG	M	1005	8,3	14,14,15	0.96	1 (7%)	15,19,21	1.76	5 (33%)
8	NAG	M	1006	8	14,14,15	0.33	0	15,19,21	0.81	1 (6%)
8	NAG	O	1001	5	14,14,15	0.20	0	15,19,21	0.60	0
8	NAG	O	1002	5	14,14,15	0.95	1 (7%)	15,19,21	0.78	0
6	HEM	P	201	1,7	28,50,50	2.11	7 (25%)	17,82,82	1.84	4 (23%)
7	OXY	P	202	6	1,1,1	0.28	0	0,0,0	0.00	-
6	HEM	Q	201	2,7	28,50,50	2.45	6 (21%)	17,82,82	2.25	6 (35%)
7	OXY	Q	202	6	1,1,1	0.26	0	0,0,0	0.00	-
8	NAG	R	1001	3	14,14,15	0.40	0	15,19,21	0.52	0
8	NAG	R	1002	8,3	14,14,15	0.53	0	15,19,21	1.58	1 (6%)
8	NAG	R	1003	8	14,14,15	1.27	2 (14%)	15,19,21	1.22	1 (6%)
8	NAG	R	1004	3	14,14,15	0.37	0	15,19,21	0.51	0
8	NAG	R	1005	8,3	14,14,15	0.82	1 (7%)	15,19,21	1.70	4 (26%)
8	NAG	R	1006	8	14,14,15	0.54	0	15,19,21	0.87	1 (6%)
8	NAG	T	1001	5	14,14,15	0.25	0	15,19,21	0.47	0
8	NAG	T	1002	5	14,14,15	0.61	1 (7%)	15,19,21	1.10	1 (6%)
6	HEM	U	201	1,7	28,50,50	2.23	6 (21%)	17,82,82	1.52	3 (17%)
7	OXY	U	202	6	1,1,1	0.29	0	0,0,0	0.00	-
6	HEM	V	201	2,7	28,50,50	2.44	7 (25%)	17,82,82	1.78	3 (17%)
7	OXY	V	202	6	1,1,1	0.30	0	0,0,0	0.00	-
8	NAG	W	1001	3	14,14,15	0.62	0	15,19,21	0.47	0
8	NAG	W	1002	3	14,14,15	0.51	0	15,19,21	1.44	1 (6%)
8	NAG	W	1003	8,3	14,14,15	0.78	1 (7%)	15,19,21	2.03	5 (33%)
8	NAG	W	1004	8	14,14,15	0.34	0	15,19,21	0.82	1 (6%)
8	NAG	Y	1001	5	14,14,15	0.38	0	15,19,21	0.53	0
8	NAG	Y	1002	5	14,14,15	0.81	1 (7%)	15,19,21	0.85	1 (6%)
6	HEM	Z	201	1,7	28,50,50	2.19	7 (25%)	17,82,82	1.78	6 (35%)
7	OXY	Z	202	6	1,1,1	0.27	0	0,0,0	0.00	-

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
6	HEM	1	201	2,7	-	0/6/54/54	0/0/8/8

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	OXY	1	202	6	-	0/0/0/0	0/0/0/0
8	NAG	2	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	2	1002	8,3	-	0/6/23/26	0/1/1/1
8	NAG	2	1003	8	-	0/6/23/26	0/1/1/1
8	NAG	2	1004	8,3	-	0/6/23/26	0/1/1/1
8	NAG	2	1005	8	-	0/6/23/26	0/1/1/1
8	NAG	4	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	4	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	A	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	A	202	6	-	0/0/0/0	0/0/0/0
6	HEM	B	201	2,7	-	2/6/54/54	0/0/8/8
7	OXY	B	202	6	-	0/0/0/0	0/0/0/0
8	NAG	C	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	C	1002	8,3	-	0/6/23/26	0/1/1/1
8	NAG	C	1003	8	-	0/6/23/26	0/1/1/1
8	NAG	C	1004	3	-	0/6/23/26	0/1/1/1
8	NAG	C	1005	8,3	-	0/6/23/26	0/1/1/1
8	NAG	C	1006	8	-	0/6/23/26	0/1/1/1
8	NAG	E	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	E	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	F	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	F	202	6	-	0/0/0/0	0/0/0/0
6	HEM	G	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	G	202	6	-	0/0/0/0	0/0/0/0
8	NAG	H	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	H	1002	3	-	0/6/23/26	0/1/1/1
8	NAG	H	1003	8,3	-	0/6/23/26	0/1/1/1
8	NAG	H	1004	8	-	0/6/23/26	0/1/1/1
8	NAG	J	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	J	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	K	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	K	202	6	-	0/0/0/0	0/0/0/0
6	HEM	L	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	L	202	6	-	0/0/0/0	0/0/0/0
8	NAG	M	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	M	1002	8,3	-	0/6/23/26	0/1/1/1
8	NAG	M	1003	8	-	0/6/23/26	0/1/1/1
8	NAG	M	1004	3	-	0/6/23/26	0/1/1/1
8	NAG	M	1005	8,3	-	0/6/23/26	0/1/1/1
8	NAG	M	1006	8	-	0/6/23/26	0/1/1/1
8	NAG	O	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	O	1002	5	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	P	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	P	202	6	-	0/0/0/0	0/0/0/0
6	HEM	Q	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	Q	202	6	-	0/0/0/0	0/0/0/0
8	NAG	R	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	R	1002	8,3	-	0/6/23/26	0/1/1/1
8	NAG	R	1003	8	-	0/6/23/26	0/1/1/1
8	NAG	R	1004	3	-	0/6/23/26	0/1/1/1
8	NAG	R	1005	8,3	-	0/6/23/26	0/1/1/1
8	NAG	R	1006	8	-	0/6/23/26	0/1/1/1
8	NAG	T	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	T	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	U	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	U	202	6	-	0/0/0/0	0/0/0/0
6	HEM	V	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	V	202	6	-	0/0/0/0	0/0/0/0
8	NAG	W	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	W	1002	3	-	0/6/23/26	0/1/1/1
8	NAG	W	1003	8,3	-	0/6/23/26	0/1/1/1
8	NAG	W	1004	8	-	0/6/23/26	0/1/1/1
8	NAG	Y	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	Y	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	Z	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	Z	202	6	-	0/0/0/0	0/0/0/0

The worst 5 of 107 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	201	HEM	C3C-C2C	-6.91	1.31	1.40
6	1	201	HEM	C3B-C2B	-6.45	1.31	1.40
6	Q	201	HEM	C3C-C2C	-6.45	1.31	1.40
6	Q	201	HEM	C3B-C2B	-6.41	1.31	1.40
6	V	201	HEM	C3C-C2C	-6.20	1.32	1.40

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	201	HEM	CAA-CBA-CGA	-5.98	102.45	112.66
6	L	201	HEM	CAD-CBD-CGD	-5.60	103.09	112.66
6	B	201	HEM	CAA-CBA-CGA	-5.48	103.30	112.66
6	B	201	HEM	CAD-CBD-CGD	-4.88	104.31	112.66
6	F	201	HEM	CMA-C3A-C4A	-4.63	121.36	128.46

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	201	HEM	C3A-C2A-CAA-CBA
6	B	201	HEM	C1A-C2A-CAA-CBA

There are no ring outliers.

38 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	201	HEM	6	0
8	2	1002	NAG	2	0
8	2	1004	NAG	1	0
8	4	1002	NAG	2	0
6	A	201	HEM	1	0
6	B	201	HEM	6	0
8	C	1002	NAG	1	0
8	C	1003	NAG	1	0
8	C	1005	NAG	1	0
8	C	1006	NAG	1	0
8	E	1002	NAG	1	0
6	F	201	HEM	2	0
6	G	201	HEM	3	0
8	H	1003	NAG	1	0
8	H	1004	NAG	2	0
8	J	1002	NAG	2	0
6	K	201	HEM	1	0
6	L	201	HEM	6	0
8	M	1001	NAG	1	0
8	M	1002	NAG	1	0
8	M	1005	NAG	1	0
8	M	1006	NAG	1	0
8	O	1002	NAG	1	0
6	P	201	HEM	2	0
6	Q	201	HEM	4	0
8	R	1002	NAG	2	0
8	R	1003	NAG	1	0
8	R	1006	NAG	1	0
8	T	1002	NAG	1	0
6	U	201	HEM	4	0
7	U	202	OXY	1	0
6	V	201	HEM	3	0
7	V	202	OXY	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	W	1002	NAG	1	0
8	W	1003	NAG	1	0
8	Y	1002	NAG	1	0
6	Z	201	HEM	2	0
7	Z	202	OXY	1	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	141/141 (100%)	-0.38	0 100 100	40, 52, 72, 81	0
1	F	141/141 (100%)	-0.36	0 100 100	49, 67, 83, 92	0
1	K	141/141 (100%)	-0.39	0 100 100	37, 53, 76, 86	0
1	P	141/141 (100%)	-0.40	0 100 100	53, 67, 91, 107	0
1	U	141/141 (100%)	-0.30	0 100 100	59, 76, 98, 100	0
1	Z	141/141 (100%)	-0.38	0 100 100	58, 72, 89, 93	0
2	1	146/146 (100%)	-0.41	1 (0%) 87 75	67, 79, 104, 138	0
2	B	146/146 (100%)	-0.38	0 100 100	39, 60, 90, 117	0
2	G	146/146 (100%)	-0.32	2 (1%) 75 57	50, 66, 97, 118	0
2	L	146/146 (100%)	-0.39	0 100 100	39, 62, 94, 120	0
2	Q	146/146 (100%)	-0.35	0 100 100	53, 69, 102, 133	0
2	V	146/146 (100%)	-0.37	0 100 100	66, 78, 105, 137	0
3	2	310/315 (98%)	-0.20	1 (0%) 93 86	63, 80, 96, 115	0
3	C	310/315 (98%)	-0.27	1 (0%) 93 86	38, 57, 75, 93	0
3	H	310/315 (98%)	-0.19	2 (0%) 89 77	56, 74, 94, 114	0
3	M	310/315 (98%)	-0.24	1 (0%) 93 86	38, 55, 79, 96	0
3	R	310/315 (98%)	-0.20	1 (0%) 93 86	65, 79, 100, 107	0
3	W	310/315 (98%)	-0.08	2 (0%) 89 77	76, 92, 112, 121	0
4	3	144/146 (98%)	-0.34	2 (1%) 75 57	60, 75, 95, 115	0
4	D	144/146 (98%)	-0.38	2 (1%) 75 57	51, 65, 84, 101	0
4	I	144/146 (98%)	-0.34	0 100 100	49, 72, 95, 111	0
4	N	144/146 (98%)	-0.30	2 (1%) 75 57	54, 68, 88, 100	0
4	S	144/146 (98%)	-0.34	0 100 100	53, 74, 94, 109	0
4	X	144/146 (98%)	-0.35	1 (0%) 87 75	61, 78, 100, 115	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	4	261/343 (76%)	-0.02	18 (6%) 18 7	74, 102, 153, 172	2 (0%)
5	E	261/343 (76%)	-0.06	13 (4%) 30 13	42, 82, 146, 155	2 (0%)
5	J	261/343 (76%)	0.24	23 (8%) 11 4	68, 110, 203, 212	2 (0%)
5	O	261/343 (76%)	-0.08	14 (5%) 26 12	43, 83, 140, 151	2 (0%)
5	T	261/343 (76%)	0.23	24 (9%) 10 3	68, 111, 197, 212	2 (0%)
5	Y	261/343 (76%)	0.26	28 (10%) 7 2	82, 111, 205, 213	2 (0%)
All	All	6012/6546 (91%)	-0.19	138 (2%) 61 39	37, 76, 138, 213	12 (0%)

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	T	293	ALA	8.8
5	T	294	GLN	7.9
5	J	118	ALA	7.6
5	J	296	GLU	7.3
5	J	219	ASN	7.2

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
6	HEM	1	201	43/43	0.95	0.24	1.28	63,68,73,76	0
6	HEM	B	201	43/43	0.96	0.23	0.57	41,50,60,64	0
8	NAG	Y	1002	14/15	0.84	0.22	0.40	81,85,88,90	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	HEM	A	201	43/43	0.95	0.21	0.35	51,55,60,62	0
6	HEM	V	201	43/43	0.96	0.21	0.24	65,69,74,76	0
6	HEM	Z	201	43/43	0.95	0.21	0.24	63,71,79,82	0
6	HEM	U	201	43/43	0.95	0.23	0.22	68,78,88,92	0
6	HEM	F	201	43/43	0.94	0.23	0.21	56,65,76,80	0
6	HEM	Q	201	43/43	0.95	0.23	0.20	58,60,62,63	0
6	HEM	G	201	43/43	0.95	0.22	0.14	53,58,64,67	0
6	HEM	P	201	43/43	0.95	0.22	0.14	63,71,79,83	0
6	HEM	K	201	43/43	0.94	0.21	0.08	43,57,69,73	0
8	NAG	2	1004	14/15	0.89	0.22	-0.09	97,97,97,97	0
6	HEM	L	201	43/43	0.95	0.21	-0.12	45,50,57,59	0
8	NAG	H	1003	14/15	0.85	0.23	-0.13	89,89,89,89	0
8	NAG	J	1002	14/15	0.89	0.17	-0.14	80,83,86,87	0
8	NAG	4	1002	14/15	0.91	0.19	-0.16	81,83,86,87	0
8	NAG	M	1005	14/15	0.84	0.21	-0.46	75,75,75,75	0
8	NAG	R	1005	14/15	0.87	0.20	-0.47	88,88,88,88	0
8	NAG	C	1005	14/15	0.87	0.18	-0.62	77,77,77,77	0
8	NAG	W	1003	14/15	0.85	0.22	-0.72	107,107,107,107	0
8	NAG	M	1006	14/15	0.81	0.22	-0.78	86,86,86,86	0
8	NAG	O	1002	14/15	0.88	0.17	-0.86	60,65,68,70	0
8	NAG	R	1006	14/15	0.79	0.22	-0.95	94,94,94,94	0
8	NAG	2	1005	14/15	0.81	0.18	-1.02	106,106,106,106	0
8	NAG	C	1006	14/15	0.83	0.17	-1.26	89,89,89,89	0
8	NAG	E	1002	14/15	0.92	0.14	-1.45	63,67,70,70	0
8	NAG	W	1004	14/15	0.74	0.23	-1.56	116,116,116,116	0
8	NAG	T	1002	14/15	0.93	0.11	-1.61	76,80,86,86	0
8	NAG	E	1001	14/15	0.85	0.42	-	103,107,112,113	0
8	NAG	H	1001	14/15	0.90	0.36	-	81,81,81,81	0
8	NAG	R	1002	14/15	0.69	0.33	-	105,105,105,105	0
8	NAG	J	1001	14/15	0.76	0.50	-	136,144,151,154	0
8	NAG	2	1001	14/15	0.87	0.37	-	101,101,101,101	0
8	NAG	H	1002	14/15	0.76	0.26	-	85,85,85,85	0
7	OXY	K	202	2/2	0.96	0.23	-	62,62,62,64	0
8	NAG	W	1001	14/15	0.88	0.39	-	101,101,101,101	0
7	OXY	A	202	2/2	0.94	0.30	-	61,61,61,62	0
7	OXY	1	202	2/2	0.99	0.21	-	69,69,69,69	0
8	NAG	C	1001	14/15	0.79	0.42	-	84,84,84,84	0
8	NAG	R	1004	14/15	0.49	0.49	-	123,123,123,123	0
7	OXY	F	202	2/2	0.97	0.29	-	72,72,72,72	0
8	NAG	M	1001	14/15	0.83	0.40	-	92,92,92,92	0
7	OXY	U	202	2/2	0.95	0.25	-	80,80,80,81	0
8	NAG	R	1001	14/15	0.83	0.38	-	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	NAG	4	1001	14/15	0.80	0.45	-	125,128,131,132	0
8	NAG	R	1003	14/15	0.83	0.37	-	112,112,112,112	0
7	OXY	Z	202	2/2	0.96	0.18	-	75,75,75,76	0
8	NAG	Y	1001	14/15	0.82	0.39	-	133,142,147,151	0
7	OXY	V	202	2/2	0.98	0.17	-	69,69,69,69	0
8	NAG	M	1004	14/15	0.70	0.44	-	116,116,116,116	0
7	OXY	Q	202	2/2	0.93	0.31	-	62,62,62,63	0
8	NAG	C	1003	14/15	0.89	0.31	-	94,94,94,94	0
8	NAG	2	1002	14/15	0.71	0.37	-	118,118,118,118	0
8	NAG	H	1004	14/15	0.79	0.22	-	98,98,98,98	0
8	NAG	O	1001	14/15	0.80	0.40	-	101,107,112,116	0
7	OXY	L	202	2/2	0.98	0.19	-	47,47,47,47	0
8	NAG	W	1002	14/15	0.66	0.34	-	112,112,112,112	0
8	NAG	C	1004	14/15	0.71	0.48	-	112,112,112,112	0
7	OXY	P	202	2/2	0.98	0.24	-	70,70,70,72	0
7	OXY	G	202	2/2	0.96	0.28	-	59,59,59,60	0
8	NAG	M	1002	14/15	0.71	0.32	-	90,90,90,90	0
8	NAG	T	1001	14/15	0.73	0.51	-	143,148,153,154	0
8	NAG	M	1003	14/15	0.80	0.40	-	97,97,97,97	0
8	NAG	C	1002	14/15	0.78	0.30	-	86,86,86,86	0
8	NAG	2	1003	14/15	0.83	0.37	-	123,123,123,123	0
7	OXY	B	202	2/2	0.97	0.22	-	49,49,49,51	0

6.5 Other polymers

There are no such residues in this entry.