



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 03:52 PM GMT

PDB ID : 1OG5  
Title : STRUCTURE OF HUMAN CYTOCHROME P450 CYP2C9  
Authors : Williams, P.A.; Cosme, J.; Ward, A.; Angove, H.C.; Matak Vinkovic, D.; Jhoti, H.  
Deposited on : 2003-04-24  
Resolution : 2.55 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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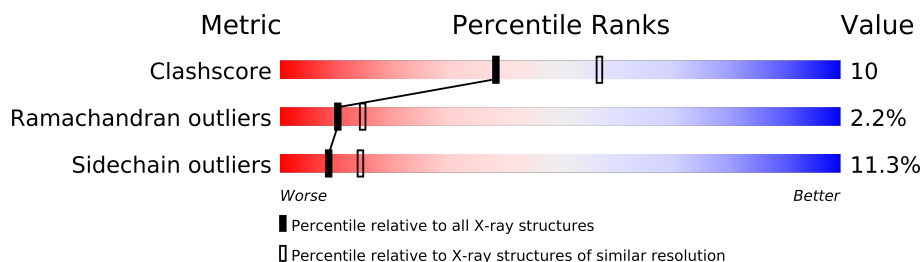
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.55 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	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	475	
1	B	475	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7939 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

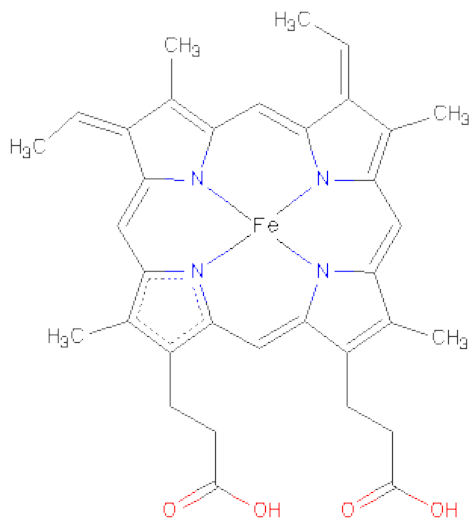
- Molecule 1 is a protein called CYTOCHROME P450 2C9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3692	2384	616	669	23			
1	B	461	Total	C	N	O	S	0	0	0
			3692	2384	616	669	23			

There are 14 discrepancies between the modelled and reference sequences:

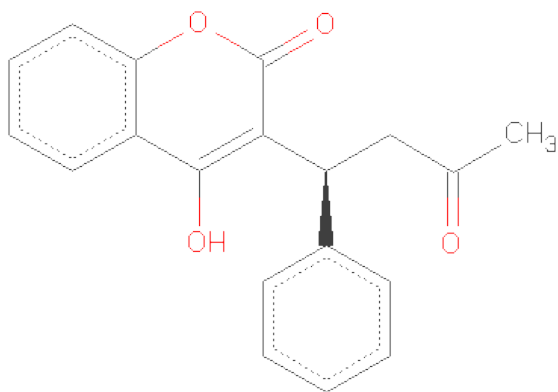
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	GLU	LYS	ENGINEERED MUTATION	UNP P11712
A	215	VAL	ILE	ENGINEERED MUTATION	UNP P11712
A	216	TYR	CYS	ENGINEERED MUTATION	UNP P11712
A	220	PRO	SER	ENGINEERED MUTATION	UNP P11712
A	221	ALA	PRO	ENGINEERED MUTATION	UNP P11712
A	222	LEU	ILE	ENGINEERED MUTATION	UNP P11712
A	223	LEU	ILE	ENGINEERED MUTATION	UNP P11712
B	206	GLU	LYS	ENGINEERED MUTATION	UNP P11712
B	215	VAL	ILE	ENGINEERED MUTATION	UNP P11712
B	216	TYR	CYS	ENGINEERED MUTATION	UNP P11712
B	220	PRO	SER	ENGINEERED MUTATION	UNP P11712
B	221	ALA	PRO	ENGINEERED MUTATION	UNP P11712
B	222	LEU	ILE	ENGINEERED MUTATION	UNP P11712
B	223	LEU	ILE	ENGINEERED MUTATION	UNP P11712

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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		

- Molecule 3 is S-WARFARIN (three-letter code: SWF) (formula:  $C_{19}H_{16}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			23	19	4		
3	B	1	Total	C	O	0	0
			23	19	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	198	Total 198	O 198	0	0
4	B	225	Total 225	O 225	0	0

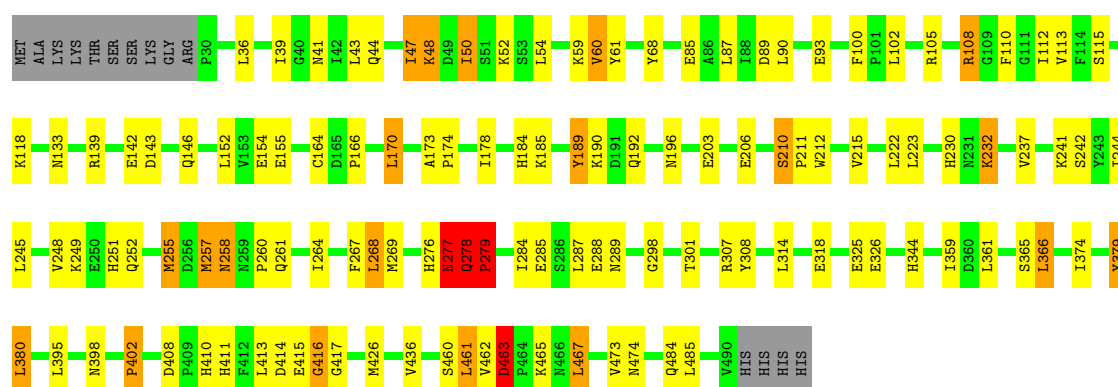
### 3 Residue-property plots

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

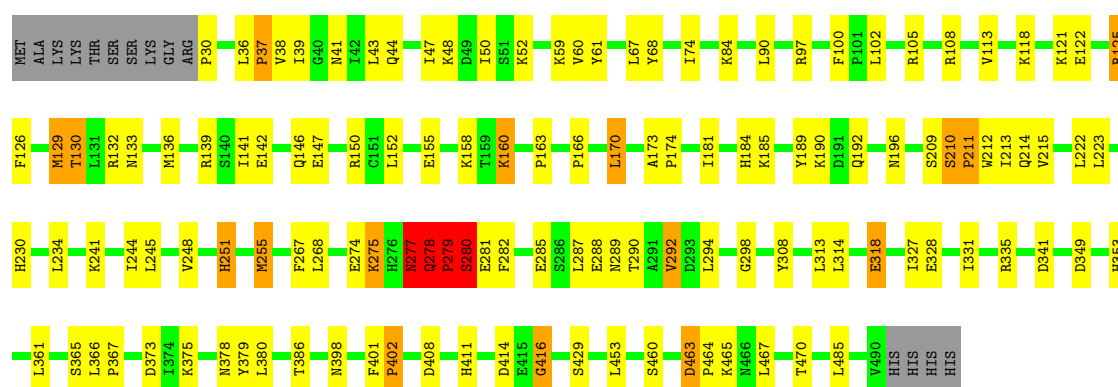
#### • Molecule 1: CYTOCHROME P450 2C9

Chain A:



#### • Molecule 1: CYTOCHROME P450 2C9

Chain B:



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.76Å 164.76Å 110.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.55	Depositor
% Data completeness (in resolution range)	99.9 (50.00-2.55)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.225 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7939	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	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: SWF, HEC

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	0.75	6/3783 (0.2%)	0.89	14/5119 (0.3%)
1	B	0.67	1/3783 (0.0%)	0.85	10/5119 (0.2%)
All	All	0.71	7/7566 (0.1%)	0.87	24/10238 (0.2%)

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	3
1	B	0	2
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	PRO	N-CD	13.92	1.67	1.47
1	A	278	GLN	C-O	7.68	1.38	1.23
1	A	277	ASN	C-O	6.64	1.35	1.23
1	B	278	GLN	N-CA	-5.71	1.34	1.46
1	A	279	PRO	N-CA	5.36	1.56	1.47
1	A	232	LYS	CD-CE	-5.17	1.38	1.51
1	A	277	ASN	N-CA	-5.14	1.36	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	279	PRO	CA-N-CD	-18.90	85.03	111.50
1	A	279	PRO	CA-N-CD	-13.83	92.14	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	GLN	C-N-CD	-13.59	90.70	120.60
1	A	277	ASN	CA-C-N	-13.09	88.41	117.20
1	A	277	ASN	N-CA-C	-12.93	76.10	111.00
1	B	277	ASN	C-N-CA	-10.45	95.58	121.70
1	A	279	PRO	N-CD-CG	-9.52	88.93	103.20
1	A	278	GLN	CA-C-N	8.92	142.08	117.10
1	A	278	GLN	O-C-N	-8.77	104.44	121.10
1	B	279	PRO	N-CD-CG	7.67	114.71	103.20
1	B	277	ASN	N-CA-C	-7.52	90.70	111.00
1	A	277	ASN	CB-CA-C	7.46	125.31	110.40
1	A	277	ASN	C-N-CA	-7.11	103.93	121.70
1	A	278	GLN	CA-C-O	-6.60	106.24	120.10
1	A	277	ASN	O-C-N	6.24	132.68	122.70
1	B	416	GLY	N-CA-C	-6.23	97.53	113.10
1	A	379	TYR	N-CA-C	6.12	127.52	111.00
1	A	257	MET	N-CA-C	-5.85	95.21	111.00
1	A	467	LEU	CA-CB-CG	5.83	128.72	115.30
1	A	416	GLY	N-CA-C	-5.71	98.84	113.10
1	B	275	LYS	N-CA-C	5.25	125.19	111.00
1	B	278	GLN	N-CA-C	5.15	124.90	111.00
1	B	278	GLN	CB-CA-C	-5.03	100.33	110.40
1	B	279	PRO	N-CA-CB	5.00	109.31	103.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	277	ASN	Mainchain
1	A	278	GLN	Mainchain,Peptide
1	B	278	GLN	Peptide
1	B	279	PRO	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3692	0	3720	73	0
1	B	3692	0	3720	72	0
2	A	43	0	32	5	0
2	B	43	0	32	3	0
3	A	23	0	16	3	0
3	B	23	0	16	5	0
4	A	198	0	0	4	0
4	B	225	0	0	1	0
All	All	7939	0	7536	147	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (147) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:125:ARG:HG3	1:B:125:ARG:HH11	0.89	1.03
1:B:278:GLN:HG2	1:B:278:GLN:O	1.23	1.03
1:B:278:GLN:CG	1:B:278:GLN:O	2.10	0.97
1:A:41:ASN:HD22	1:A:68:TYR:H	1.11	0.96
1:B:41:ASN:HD22	1:B:68:TYR:H	1.00	0.96
1:B:125:ARG:HG3	1:B:125:ARG:NH1	1.69	0.92
1:B:125:ARG:HH11	1:B:125:ARG:CG	1.82	0.90
1:A:203:GLU:OE2	1:A:232:LYS:CE	2.25	0.85
1:A:277:ASN:O	1:A:278:GLN:CB	2.24	0.84
1:A:203:GLU:OE2	1:A:232:LYS:HE2	1.77	0.84
1:A:277:ASN:O	1:A:278:GLN:HB3	1.75	0.84
1:A:301:THR:HG23	1:A:361:LEU:HD23	1.60	0.83
1:B:133:ASN:HD21	1:B:142:GLU:H	1.32	0.78
1:A:155:GLU:HG3	1:A:189:TYR:CD1	2.21	0.76
1:B:41:ASN:HD22	1:B:68:TYR:N	1.83	0.74
1:B:41:ASN:ND2	1:B:68:TYR:H	1.80	0.73
1:A:241:LYS:HE2	1:A:289:ASN:ND2	2.04	0.73
1:A:166:PRO:HB2	1:A:170:LEU:HD22	1.71	0.72
1:B:126:PHE:O	1:B:130:THR:HG23	1.89	0.72
1:A:113:VAL:HG12	3:A:502:SWF:H17	1.71	0.72
1:A:133:ASN:HD21	1:A:142:GLU:H	1.37	0.72
1:B:241:LYS:NZ	1:B:289:ASN:HD21	1.88	0.71
1:A:155:GLU:HG3	1:A:189:TYR:HD1	1.54	0.70
1:A:414:ASP:OD2	1:A:416:GLY:O	2.09	0.70
1:A:365:SER:OG	2:A:501:HEC:HBA1	1.92	0.69
1:A:178:ILE:CD1	4:A:2185:HOH:O	2.43	0.67
1:A:307:ARG:NH2	4:A:2109:HOH:O	2.29	0.64
1:A:105:ARG:HG3	1:A:223:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:113:VAL:CG1	3:A:502:SWF:H17	2.27	0.63
1:B:210:SER:OG	1:B:212:TRP:CD1	2.52	0.63
1:B:212:TRP:O	1:B:212:TRP:CE3	2.51	0.63
1:A:178:ILE:HD11	4:A:2185:HOH:O	1.99	0.62
1:B:113:VAL:HG12	3:B:502:SWF:H17	1.79	0.62
1:B:244:ILE:O	1:B:248:VAL:HG13	1.99	0.62
1:A:325:GLU:OE1	1:A:326:GLU:N	2.34	0.61
1:A:184:HIS:ND1	1:A:261:GLN:HB3	2.14	0.61
1:A:50:ILE:HG13	1:A:50:ILE:O	2.00	0.60
1:B:251:HIS:O	1:B:255:MET:HB2	2.01	0.60
1:B:274:GLU:OE1	1:B:280:SER:HB2	2.03	0.59
1:B:155:GLU:HG3	1:B:189:TYR:CD1	2.39	0.58
1:A:133:ASN:ND2	1:A:142:GLU:H	2.01	0.57
1:B:133:ASN:ND2	1:B:142:GLU:H	2.00	0.57
1:A:36:LEU:HD12	1:A:39:ILE:HD11	1.87	0.57
1:B:408:ASP:HB3	1:B:411:HIS:HD2	1.68	0.57
1:A:241:LYS:HE2	1:A:289:ASN:HD22	1.66	0.57
1:A:278:GLN:C	1:A:279:PRO:O	2.43	0.57
1:B:463:ASP:OD1	1:B:464:PRO:HD2	2.05	0.57
1:A:203:GLU:OE2	1:A:232:LYS:NZ	2.38	0.57
1:A:462:VAL:O	1:A:463:ASP:HB3	2.05	0.57
1:A:325:GLU:C	1:A:325:GLU:OE1	2.43	0.56
1:A:93:GLU:HG2	1:A:374:ILE:HD13	1.85	0.56
1:A:41:ASN:HD22	1:A:68:TYR:N	1.93	0.56
1:B:288:GLU:O	1:B:292:VAL:HG13	2.05	0.56
1:B:108:ARG:HG3	1:B:234:LEU:HD21	1.88	0.56
1:B:100:PHE:HB2	3:B:502:SWF:H4C1	1.87	0.56
1:B:408:ASP:HB3	1:B:411:HIS:CD2	2.41	0.56
1:B:241:LYS:HE2	1:B:289:ASN:ND2	2.20	0.55
1:B:113:VAL:CG1	3:B:502:SWF:H17	2.36	0.55
1:A:50:ILE:O	1:A:54:LEU:HG	2.06	0.55
1:A:41:ASN:ND2	1:A:68:TYR:H	1.92	0.55
2:A:501:HEC:HHD	2:A:501:HEC:HBC2	1.89	0.54
1:A:184:HIS:O	1:A:184:HIS:CD2	2.60	0.54
1:A:277:ASN:O	1:A:278:GLN:HB2	2.07	0.54
1:B:335:ARG:NH2	1:B:341:ASP:OD1	2.42	0.53
1:A:85:GLU:O	1:A:89:ASP:HB2	2.09	0.53
1:B:313:LEU:HD13	1:B:453:LEU:HD11	1.91	0.53
1:A:192:GLN:HE21	1:A:196:ASN:HD21	1.56	0.53
1:B:267:PHE:CE2	1:B:287:LEU:HB2	2.45	0.52
1:B:36:LEU:HD12	1:B:39:ILE:HD11	1.91	0.52
1:A:108:ARG:CG	1:A:108:ARG:HH11	2.23	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:184:HIS:HD2	1:A:184:HIS:O	1.92	0.52
1:A:173:ALA:HB3	1:A:174:PRO:HD3	1.92	0.51
1:B:166:PRO:HB2	1:B:170:LEU:HD22	1.93	0.51
1:B:414:ASP:OD2	1:B:416:GLY:O	2.28	0.50
1:B:125:ARG:NH1	1:B:125:ARG:CG	2.53	0.50
1:A:249:LYS:HA	1:A:252:GLN:HE21	1.76	0.50
1:A:284:ILE:O	1:A:288:GLU:HG3	2.11	0.50
1:A:244:ILE:O	1:A:248:VAL:HG13	2.11	0.49
1:A:426:MET:HA	4:A:2173:HOH:O	2.12	0.49
1:B:108:ARG:HG3	1:B:234:LEU:CD2	2.42	0.49
1:A:215:VAL:HG12	1:A:222:LEU:HD12	1.95	0.48
1:B:118:LYS:CE	1:B:122:GLU:OE1	2.61	0.48
1:A:100:PHE:HB2	3:A:502:SWF:O23	2.12	0.48
1:B:314:LEU:HD22	1:B:460:SER:HB2	1.94	0.48
1:B:155:GLU:HG3	1:B:189:TYR:HD1	1.78	0.48
1:A:379:TYR:O	1:A:380:LEU:HB3	2.14	0.48
1:B:209:SER:O	1:B:211:PRO:HD3	2.13	0.48
1:B:142:GLU:O	1:B:146:GLN:HG3	2.14	0.48
1:A:251:HIS:O	1:A:255:MET:HB2	2.14	0.48
1:A:359:ILE:HD12	1:A:361:LEU:HD13	1.96	0.48
1:B:105:ARG:HG3	1:B:223:LEU:HD13	1.95	0.47
1:B:173:ALA:HB3	1:B:174:PRO:HD3	1.96	0.47
1:A:314:LEU:HD22	1:A:460:SER:HB2	1.97	0.47
1:A:298:GLY:HA2	2:A:501:HEC:C2C	2.44	0.47
1:B:118:LYS:HE3	1:B:122:GLU:OE1	2.14	0.47
1:B:100:PHE:HB2	3:B:502:SWF:O23	2.15	0.47
1:A:408:ASP:O	1:A:411:HIS:HD2	1.98	0.47
1:A:264:ILE:HG22	1:A:268:LEU:HD22	1.96	0.47
1:A:142:GLU:O	1:A:146:GLN:HG3	2.15	0.47
1:B:298:GLY:HA2	2:B:501:HEC:C2C	2.44	0.46
1:A:155:GLU:HG3	1:A:189:TYR:CE1	2.50	0.46
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.80	0.46
1:B:129:MET:SD	1:B:132:ARG:CZ	3.03	0.46
1:A:366:LEU:HB2	2:A:501:HEC:HAA2	1.96	0.46
1:A:461:LEU:HD11	1:A:484:GLN:HB2	1.97	0.46
1:A:184:HIS:CE1	1:A:261:GLN:HB3	2.50	0.46
1:B:158:LYS:O	1:B:160:LYS:HG2	2.16	0.45
1:B:401:PHE:HB3	1:B:411:HIS:ND1	2.32	0.45
1:B:133:ASN:HD22	1:B:141:ILE:HB	1.81	0.45
1:B:318:GLU:HB2	4:B:2125:HOH:O	2.16	0.45
1:A:410:HIS:ND1	1:A:413:LEU:HD12	2.32	0.44
1:B:215:VAL:HG12	1:B:222:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:257:MET:O	1:A:258:ASN:CB	2.65	0.44
1:B:30:PRO:HG3	1:B:379:TYR:HB3	1.99	0.44
1:B:290:THR:O	1:B:294:LEU:HG	2.18	0.44
1:B:102:LEU:HD12	3:B:502:SWF:H1C2	2.00	0.44
2:B:501:HEC:HHD	2:B:501:HEC:HBC2	1.98	0.44
1:B:327:ILE:O	1:B:331:ILE:O	2.36	0.43
1:B:74:ILE:HD12	1:B:386:THR:HB	2.00	0.43
1:B:349:ASP:O	1:B:353:HIS:HD2	2.01	0.43
1:A:110:PHE:HB3	1:A:115:SER:OG	2.18	0.43
1:B:375:LYS:HA	1:B:379:TYR:O	2.18	0.43
1:A:260:PRO:HB3	1:A:269:MET:HE1	1.99	0.43
1:B:274:GLU:O	1:B:277:ASN:O	2.37	0.43
1:B:365:SER:OG	2:B:501:HEC:HAA2	2.18	0.43
1:A:267:PHE:CG	1:A:287:LEU:HD13	2.54	0.43
1:B:280:SER:OG	1:B:282:PHE:N	2.50	0.42
1:B:241:LYS:HZ3	1:B:289:ASN:HD21	1.62	0.42
1:B:60:VAL:HG22	1:B:61:TYR:CD2	2.54	0.42
1:A:112:ILE:HD11	1:A:436:VAL:HG21	2.02	0.42
1:A:301:THR:HG22	2:A:501:HEC:HBB3	2.01	0.42
1:A:276:HIS:C	1:A:277:ASN:O	2.47	0.42
1:B:97:ARG:HD3	1:B:367:PRO:O	2.20	0.42
1:B:241:LYS:CE	1:B:289:ASN:ND2	2.83	0.41
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.35	0.41
1:B:192:GLN:HE21	1:B:196:ASN:ND2	2.18	0.41
1:A:237:VAL:HG12	1:A:241:LYS:HE3	2.01	0.41
1:A:314:LEU:HD11	1:A:485:LEU:HB3	2.02	0.41
1:B:147:GLU:HA	1:B:150:ARG:NH2	2.35	0.41
1:A:474:ASN:HA	1:A:474:ASN:HD22	1.65	0.41
1:B:314:LEU:HD11	1:B:485:LEU:HB3	2.01	0.41
1:B:401:PHE:HB3	1:B:411:HIS:CE1	2.56	0.41
1:B:41:ASN:ND2	1:B:68:TYR:N	2.55	0.41
1:B:136:MET:CE	1:B:181:ILE:HG23	2.51	0.41
1:A:210:SER:OG	1:A:212:TRP:NE1	2.46	0.41
1:B:281:GLU:HA	1:B:281:GLU:OE1	2.21	0.40
1:A:60:VAL:HG22	1:A:61:TYR:CD2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/475 (97%)	426 (93%)	23 (5%)	10 (2%)	10	15
1	B	459/475 (97%)	423 (92%)	26 (6%)	10 (2%)	10	15
All	All	918/950 (97%)	849 (92%)	49 (5%)	20 (2%)	10	15

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	PRO
1	A	230	HIS
1	A	258	ASN
1	A	402	PRO
1	B	230	HIS
1	B	463	ASP
1	B	37	PRO
1	B	275	LYS
1	B	280	SER
1	A	48	LYS
1	A	189	TYR
1	A	278	GLN
1	B	48	LYS
1	A	463	ASP
1	B	279	PRO
1	B	429	SER
1	B	47	ILE
1	A	47	ILE
1	A	417	GLY
1	B	402	PRO

### 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	416/428 (97%)	371 (89%)	45 (11%)	9	16
1	B	416/428 (97%)	367 (88%)	49 (12%)	8	13
All	All	832/856 (97%)	738 (89%)	94 (11%)	9	14

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	44	GLN
1	A	47	ILE
1	A	48	LYS
1	A	50	ILE
1	A	52	LYS
1	A	59	LYS
1	A	60	VAL
1	A	87	LEU
1	A	90	LEU
1	A	102	LEU
1	A	108	ARG
1	A	118	LYS
1	A	139	ARG
1	A	143	ASP
1	A	152	LEU
1	A	154	GLU
1	A	164	CYS
1	A	170	LEU
1	A	185	LYS
1	A	190	LYS
1	A	206	GLU
1	A	210	SER
1	A	211	PRO
1	A	242	SER
1	A	245	LEU
1	A	255	MET
1	A	268	LEU
1	A	277	ASN
1	A	278	GLN
1	A	285	GLU
1	A	308	TYR
1	A	318	GLU
1	A	344	HIS

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Mol	Chain	Res	Type
1	A	366	LEU
1	A	380	LEU
1	A	395	LEU
1	A	398	ASN
1	A	402	PRO
1	A	415	GLU
1	A	461	LEU
1	A	463	ASP
1	A	465	LYS
1	A	467	LEU
1	A	473	VAL
1	B	37	PRO
1	B	38	VAL
1	B	43	LEU
1	B	44	GLN
1	B	50	ILE
1	B	52	LYS
1	B	59	LYS
1	B	67	LEU
1	B	84	LYS
1	B	90	LEU
1	B	121	LYS
1	B	125	ARG
1	B	129	MET
1	B	130	THR
1	B	139	ARG
1	B	152	LEU
1	B	160	LYS
1	B	163	PRO
1	B	170	LEU
1	B	184	HIS
1	B	185	LYS
1	B	190	LYS
1	B	210	SER
1	B	211	PRO
1	B	213	ILE
1	B	214	GLN
1	B	245	LEU
1	B	251	HIS
1	B	255	MET
1	B	268	LEU
1	B	277	ASN

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Mol	Chain	Res	Type
1	B	278	GLN
1	B	279	PRO
1	B	280	SER
1	B	285	GLU
1	B	292	VAL
1	B	308	TYR
1	B	318	GLU
1	B	328	GLU
1	B	361	LEU
1	B	366	LEU
1	B	373	ASP
1	B	378	ASN
1	B	380	LEU
1	B	398	ASN
1	B	402	PRO
1	B	465	LYS
1	B	467	LEU
1	B	470	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	44	GLN
1	A	133	ASN
1	A	184	HIS
1	A	196	ASN
1	A	202	ASN
1	A	204	ASN
1	A	236	ASN
1	A	252	GLN
1	A	259	ASN
1	A	289	ASN
1	A	316	HIS
1	A	324	GLN
1	A	378	ASN
1	A	398	ASN
1	A	411	HIS
1	A	418	ASN
1	A	474	ASN
1	B	41	ASN
1	B	44	GLN

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Mol	Chain	Res	Type
1	B	133	ASN
1	B	146	GLN
1	B	196	ASN
1	B	202	ASN
1	B	204	ASN
1	B	236	ASN
1	B	252	GLN
1	B	276	HIS
1	B	289	ASN
1	B	324	GLN
1	B	334	ASN
1	B	353	HIS
1	B	368	HIS
1	B	411	HIS
1	B	454	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEC	A	501	1	50,50,50	2.62	12 (24%)	56,82,82	1.58	11 (19%)
3	SWF	A	502	-	25,25,25	3.71	16 (64%)	33,35,35	3.38	13 (39%)
2	HEC	B	501	1	50,50,50	3.01	16 (32%)	56,82,82	1.32	7 (12%)
3	SWF	B	502	-	25,25,25	3.58	14 (56%)	33,35,35	3.16	10 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	A	501	1	-	0/10/54/54	0/0/8/8
3	SWF	A	502	-	-	0/12/12/12	0/1/3/3
2	HEC	B	501	1	-	0/10/54/54	0/0/8/8
3	SWF	B	502	-	-	0/12/12/12	0/1/3/3

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	SWF	O21-C22	12.75	1.39	1.33
3	B	502	SWF	O21-C22	11.33	1.38	1.33
2	B	501	HEC	C1C-C2C	8.80	1.51	1.40
2	B	501	HEC	C3C-CAC	7.89	1.51	1.35
2	A	501	HEC	C3C-CAC	7.79	1.51	1.35
2	A	501	HEC	C1C-C2C	7.56	1.49	1.40
2	A	501	HEC	C3B-CAB	6.74	1.49	1.35
3	B	502	SWF	C12-C5	6.57	1.58	1.52
2	B	501	HEC	C3C-C4C	6.57	1.49	1.41
2	B	501	HEC	C3B-CAB	6.45	1.48	1.35
2	B	501	HEC	C1B-C2B	6.25	1.48	1.40
2	A	501	HEC	C3C-C4C	6.04	1.49	1.41
3	B	502	SWF	C15-C20	5.90	1.49	1.41
2	B	501	HEC	C3B-C4B	5.83	1.48	1.41
3	A	502	SWF	C15-C20	5.82	1.49	1.41
3	A	502	SWF	C11-C6	5.29	1.48	1.39
2	A	501	HEC	C1B-C2B	5.21	1.46	1.40
3	A	502	SWF	C12-C5	5.17	1.57	1.52
2	B	501	HEC	FE-NC	5.16	2.14	1.92
3	B	502	SWF	C11-C6	5.12	1.47	1.39
2	A	501	HEC	FE-NC	4.30	2.10	1.92
2	B	501	HEC	FE-NA	4.21	2.10	1.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEC	FE-NA	4.20	2.10	1.92
2	B	501	HEC	CBB-CAB	-4.15	1.31	1.49
2	A	501	HEC	C3B-C4B	4.06	1.46	1.41
2	A	501	HEC	CBB-CAB	-3.95	1.32	1.49
3	B	502	SWF	C7-C6	3.89	1.45	1.39
2	B	501	HEC	C1A-NA	3.83	1.42	1.37
3	A	502	SWF	C7-C6	3.77	1.45	1.39
2	A	501	HEC	CBC-CAC	-3.55	1.34	1.49
2	B	501	HEC	CBC-CAC	-3.51	1.34	1.49
2	B	501	HEC	FE-NB	3.34	2.06	1.92
3	A	502	SWF	C4-C2	3.09	1.55	1.50
3	B	502	SWF	C13-C15	2.87	1.49	1.43
2	B	501	HEC	C1D-C2D	2.84	1.43	1.40
3	A	502	SWF	C19-C20	2.77	1.44	1.38
3	B	502	SWF	C18-C19	2.65	1.42	1.36
3	A	502	SWF	C8-C7	2.60	1.45	1.39
3	A	502	SWF	C13-C15	2.60	1.49	1.43
3	B	502	SWF	C9-C8	2.56	1.45	1.37
2	B	501	HEC	FE-ND	2.55	2.03	1.92
3	B	502	SWF	C18-C17	2.54	1.45	1.37
3	A	502	SWF	C9-C8	2.54	1.45	1.37
3	A	502	SWF	C18-C19	2.53	1.42	1.36
3	B	502	SWF	C19-C20	2.47	1.43	1.38
3	A	502	SWF	C4-C5	2.46	1.60	1.53
3	A	502	SWF	C18-C17	2.35	1.44	1.37
3	B	502	SWF	C4-C5	2.30	1.59	1.53
3	B	502	SWF	C8-C7	2.23	1.44	1.39
2	A	501	HEC	FE-NB	2.22	2.01	1.92
2	B	501	HEC	CBD-CGD	2.14	1.56	1.50
3	B	502	SWF	C4-C2	2.13	1.54	1.50
2	B	501	HEC	C1C-NC	2.13	1.40	1.36
2	A	501	HEC	C4A-C3A	2.11	1.50	1.43
3	A	502	SWF	C10-C11	2.08	1.43	1.39
3	B	502	SWF	C17-C16	2.05	1.41	1.36
3	A	502	SWF	C10-C9	2.04	1.43	1.37
3	A	502	SWF	C22-C12	2.02	1.47	1.40

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	SWF	C22-O21-C20	10.53	121.70	118.14
3	A	502	SWF	O21-C22-C12	-9.99	122.62	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	SWF	C22-O21-C20	9.71	121.42	118.14
3	B	502	SWF	O21-C22-C12	-8.90	122.97	125.82
3	A	502	SWF	C12-C5-C6	-8.11	99.90	111.67
3	B	502	SWF	C12-C5-C6	-7.02	101.47	111.67
3	A	502	SWF	O21-C20-C19	4.52	121.57	115.99
3	A	502	SWF	C1-C2-C4	4.52	123.36	116.63
3	B	502	SWF	O21-C20-C19	4.29	121.28	115.99
2	B	501	HEC	CMB-C2B-C3B	4.04	130.18	125.72
2	A	501	HEC	CMB-C2B-C3B	3.70	129.80	125.72
2	A	501	HEC	C4A-C3A-C2A	-3.64	104.58	106.89
2	B	501	HEC	CAA-C2A-C1A	3.63	131.22	124.67
3	A	502	SWF	C19-C20-C15	-3.51	119.37	123.12
3	A	502	SWF	C16-C15-C20	3.48	120.56	116.30
3	B	502	SWF	C16-C15-C20	3.46	120.53	116.30
2	A	501	HEC	CAA-C2A-C1A	-3.44	118.47	124.67
3	B	502	SWF	C19-C20-C15	-3.39	119.50	123.12
2	B	501	HEC	CMB-C2B-C1B	-3.36	123.45	128.62
2	A	501	HEC	CMC-C2C-C3C	3.33	129.40	125.72
2	A	501	HEC	CMB-C2B-C1B	-3.12	123.82	128.62
3	B	502	SWF	C1-C2-C4	3.08	121.23	116.63
3	B	502	SWF	C12-C13-C15	-3.00	119.41	121.78
3	A	502	SWF	C4-C5-C12	2.98	117.21	111.34
2	A	501	HEC	C2A-C1A-NA	2.82	111.75	109.64
3	A	502	SWF	C12-C13-C15	-2.80	119.57	121.78
2	A	501	HEC	CMA-C3A-C2A	2.67	129.97	124.94
3	A	502	SWF	C13-C12-C5	-2.65	117.26	121.31
2	A	501	HEC	CMC-C2C-C1C	-2.55	124.70	128.62
2	A	501	HEC	C3A-C4A-NA	2.55	111.33	109.41
3	B	502	SWF	C4-C5-C12	2.53	116.33	111.34
2	B	501	HEC	CBA-CAA-C2A	2.53	117.08	112.35
2	B	501	HEC	CMC-C2C-C3C	2.34	128.30	125.72
2	A	501	HEC	CMD-C2D-C1D	-2.30	125.09	128.62
3	A	502	SWF	O21-C20-C15	-2.22	119.06	121.36
3	A	502	SWF	O14-C13-C15	2.15	120.72	116.55
2	B	501	HEC	CAA-C2A-C3A	-2.12	122.96	129.00
2	B	501	HEC	C3C-C2C-C1C	-2.08	105.68	107.07
3	B	502	SWF	O21-C20-C15	-2.06	119.22	121.36
2	A	501	HEC	C3B-C4B-NB	-2.05	108.56	111.52
3	A	502	SWF	C22-C12-C5	2.03	124.42	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 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.