



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:25 am GMT

PDB ID : 1Z10  
Title : Crystal Structure of Human Microsomal P450 2A6 with Coumarin Bound  
Authors : Yano, J.K.; Hsu, M.H.; Griffin, K.J.; Stout, C.D.; Johnson, E.F.  
Deposited on : 2005-03-02  
Resolution : 1.90 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
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) : recalc28949

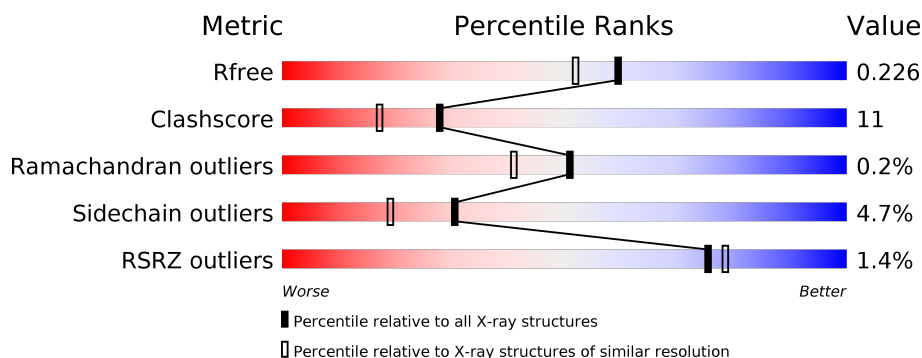
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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. 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	476	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>••</div> </div> </div>
1	B	476	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>••</div> </div> </div>
1	C	476	<div> <div></div> <div> <div></div> <div>78%</div> <div>16%</div> <div>••</div> </div> </div>
1	D	476	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	COU	C	501	-	-	-	X
3	COU	D	501	-	-	-	X
4	GOL	B	900	-	X	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16075 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 cytochrome P450, family 2, subfamily A, polypeptide 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	1	0
			3768	2420	651	679	18			
1	B	465	Total	C	N	O	S	0	0	0
			3767	2418	653	678	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	SEE REMARK 999	UNP P11509
A	24	ALA	-	SEE REMARK 999	UNP P11509
A	25	LYS	-	SEE REMARK 999	UNP P11509
A	26	LYS	-	SEE REMARK 999	UNP P11509
A	27	THR	-	SEE REMARK 999	UNP P11509
A	28	SER	-	SEE REMARK 999	UNP P11509
A	495	HIS	-	EXPRESSION TAG	UNP P11509
A	496	HIS	-	EXPRESSION TAG	UNP P11509
A	497	HIS	-	EXPRESSION TAG	UNP P11509
A	498	HIS	-	EXPRESSION TAG	UNP P11509
B	23	MET	-	SEE REMARK 999	UNP P11509
B	24	ALA	-	SEE REMARK 999	UNP P11509
B	25	LYS	-	SEE REMARK 999	UNP P11509
B	26	LYS	-	SEE REMARK 999	UNP P11509
B	27	THR	-	SEE REMARK 999	UNP P11509
B	28	SER	-	SEE REMARK 999	UNP P11509
B	495	HIS	-	EXPRESSION TAG	UNP P11509
B	496	HIS	-	EXPRESSION TAG	UNP P11509
B	497	HIS	-	EXPRESSION TAG	UNP P11509
B	498	HIS	-	EXPRESSION TAG	UNP P11509
C	23	MET	-	SEE REMARK 999	UNP P11509

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	ALA	-	SEE REMARK 999	UNP P11509
C	25	LYS	-	SEE REMARK 999	UNP P11509
C	26	LYS	-	SEE REMARK 999	UNP P11509
C	27	THR	-	SEE REMARK 999	UNP P11509
C	28	SER	-	SEE REMARK 999	UNP P11509
C	495	HIS	-	EXPRESSION TAG	UNP P11509
C	496	HIS	-	EXPRESSION TAG	UNP P11509
C	497	HIS	-	EXPRESSION TAG	UNP P11509
C	498	HIS	-	EXPRESSION TAG	UNP P11509
D	23	MET	-	SEE REMARK 999	UNP P11509
D	24	ALA	-	SEE REMARK 999	UNP P11509
D	25	LYS	-	SEE REMARK 999	UNP P11509
D	26	LYS	-	SEE REMARK 999	UNP P11509
D	27	THR	-	SEE REMARK 999	UNP P11509
D	28	SER	-	SEE REMARK 999	UNP P11509
D	495	HIS	-	EXPRESSION TAG	UNP P11509
D	496	HIS	-	EXPRESSION TAG	UNP P11509
D	497	HIS	-	EXPRESSION TAG	UNP P11509
D	498	HIS	-	EXPRESSION TAG	UNP P11509

- # HEM
- 
- The diagram illustrates the chemical structure of Hemoglobin (HEM). It features a central iron atom (Fe) coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with various side chains, including vinyl groups (CH=CH<sub>2</sub>), methyl groups (CH<sub>3</sub>), and ethyl groups (CH<sub>2</sub>CH<sub>3</sub>). The heme group is shown as a central iron atom coordinated by four nitrogen atoms, with various side chains and a heme group. The structure is labeled with various atoms and bonds, including C, N, O, and Fe, and is color-coded to show different components.

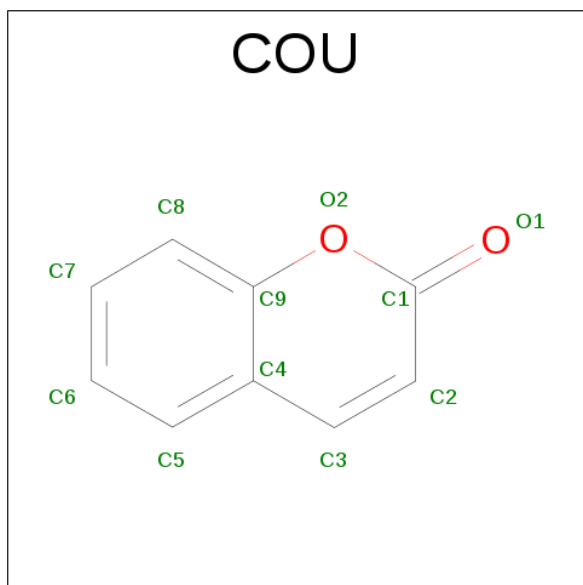
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0



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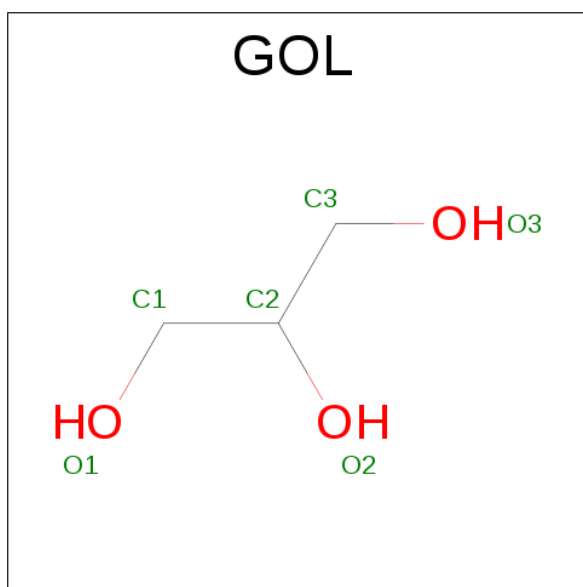
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is COUMARIN (three-letter code: COU) (formula:  $C_9H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O		
			11	9	2		
3	B	1	Total	C	O		
			11	9	2		
3	C	1	Total	C	O		
			11	9	2		
3	D	1	Total	C	O		
			11	9	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		

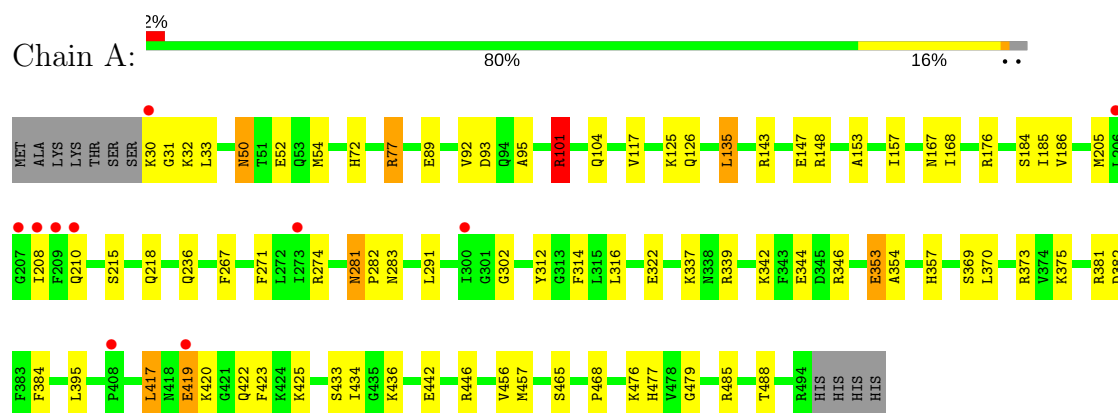
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	224	Total	O	0	0
			224	224		
5	B	140	Total	O	0	0
			140	140		
5	C	237	Total	O	0	0
			237	237		
5	D	215	Total	O	0	0
			215	215		

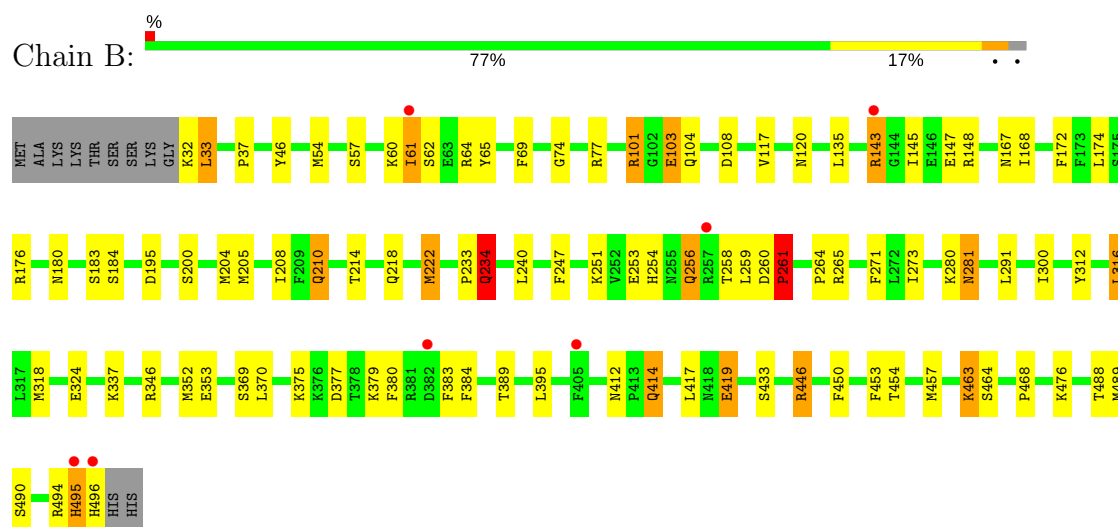
### 3 Residue-property plots

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.

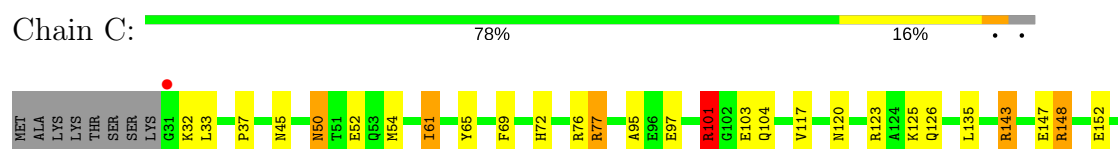
- Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6



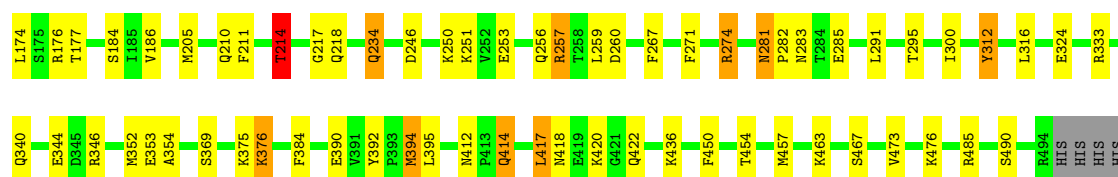
- Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6



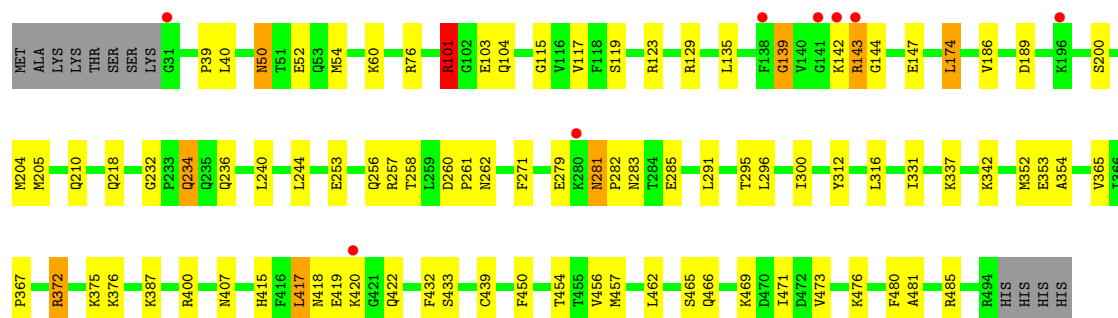
- Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6







- Molecule 1: cytochrome P450, family 2, subfamily A, polypeptide 6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.61Å 157.59Å 103.54Å 90.00° 92.25° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 47.43 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.8 (50.00-1.90) 92.9 (47.43-1.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.194 , 0.230 0.190 , 0.226	Depositor DCC
$R_{free}$ test set	8261 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, COU, HEM

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	0.86	0/3859	0.90	5/5197 (0.1%)
1	B	0.81	2/3860 (0.1%)	0.89	6/5200 (0.1%)
1	C	0.87	2/3842 (0.1%)	0.91	6/5175 (0.1%)
1	D	0.83	0/3842	0.93	7/5175 (0.1%)
All	All	0.84	4/15403 (0.0%)	0.91	24/20747 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	394	MET	SD-CE	-8.21	1.31	1.77
1	C	214	THR	CB-CG2	-5.98	1.32	1.52
1	B	222	MET	SD-CE	-5.35	1.47	1.77
1	B	103	GLU	CG-CD	5.20	1.59	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	NE-CZ-NH1	16.58	128.59	120.30
1	B	101	ARG	NE-CZ-NH2	-16.33	112.13	120.30
1	A	101	ARG	NE-CZ-NH2	-15.67	112.47	120.30
1	D	372	ARG	NE-CZ-NH2	-15.48	112.56	120.30
1	C	101	ARG	NE-CZ-NH2	-15.13	112.73	120.30
1	C	101	ARG	NE-CZ-NH1	14.08	127.34	120.30
1	D	101	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	D	372	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	D	101	ARG	NE-CZ-NH1	11.67	126.14	120.30
1	B	101	ARG	NE-CZ-NH1	11.40	126.00	120.30
1	D	104	GLN	N-CA-C	-6.17	94.34	111.00
1	D	372	ARG	CG-CD-NE	-6.08	99.04	111.80
1	C	104	GLN	N-CA-C	-5.97	94.87	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ARG	CD-NE-CZ	5.82	131.74	123.60
1	B	33	LEU	CA-CB-CG	5.50	127.96	115.30
1	B	104	GLN	N-CA-C	-5.48	96.21	111.00
1	A	104	GLN	N-CA-C	-5.35	96.57	111.00
1	A	479	GLY	N-CA-C	-5.20	100.11	113.10
1	D	139	GLY	N-CA-C	5.16	125.99	113.10
1	C	274	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	C	101	ARG	CD-NE-CZ	5.08	130.72	123.60
1	B	316	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	214	THR	N-CA-CB	-5.04	100.72	110.30
1	B	234	GLN	CA-CB-CG	5.00	124.41	113.40

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	3768	0	3757	70	0
1	B	3767	0	3745	98	0
1	C	3751	0	3734	99	0
1	D	3751	0	3734	71	0
2	A	43	0	30	4	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	11	0	6	0	0
3	B	11	0	6	0	0
3	C	11	0	6	0	0
3	D	11	0	6	0	0
4	B	6	0	5	3	0
5	A	224	0	0	3	0
5	B	140	0	0	2	0
5	C	237	0	0	5	0
5	D	215	0	0	5	0
All	All	16075	0	15119	339	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 11.

All (339) 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)
4:B:900:GOL:O1	4:B:900:GOL:C1	1.71	1.35
1:B:205:MET:HE1	1:B:300:ILE:HA	1.28	1.12
1:B:208:ILE:HD11	1:B:240:LEU:HB2	1.17	1.08
1:C:418:ASN:HD22	1:C:422:GLN:HB2	1.15	1.08
1:D:189:ASP:HB2	5:D:695:HOH:O	1.55	1.06
1:C:77:ARG:HG2	1:C:77:ARG:HH11	1.12	1.04
1:D:253:GLU:HG2	1:D:257:ARG:NH2	1.74	1.02
1:C:234:GLN:H	1:C:234:GLN:HE21	1.05	1.01
1:D:139:GLY:HA2	1:D:142:LYS:HE3	1.42	0.99
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.26	0.98
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.45	0.97
1:B:101:ARG:H	1:B:120:ASN:ND2	1.65	0.94
1:C:45:ASN:HD22	1:C:72:HIS:H	1.17	0.91
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.34	0.91
1:B:208:ILE:HD11	1:B:240:LEU:CB	2.01	0.91
1:B:205:MET:CE	1:B:300:ILE:HA	2.02	0.90
1:B:234:GLN:HE21	1:B:234:GLN:H	1.20	0.90
1:C:101:ARG:H	1:C:120:ASN:ND2	1.70	0.90
1:D:253:GLU:HG2	1:D:257:ARG:HH21	1.34	0.89
1:B:352:MET:HE3	1:B:454:THR:HG22	1.55	0.87
1:D:54:MET:HG3	1:D:218:GLN:HE21	1.40	0.86
1:B:446:ARG:HG3	1:B:446:ARG:HH11	1.41	0.85
1:A:54:MET:HG3	1:A:218:GLN:HE21	1.37	0.85
1:A:322:GLU:N	1:A:322:GLU:OE2	2.08	0.85
1:B:234:GLN:NE2	1:B:234:GLN:H	1.73	0.85
1:A:420:LYS:HB2	1:A:422:GLN:HE21	1.42	0.85
1:B:54:MET:HG3	1:B:218:GLN:HE21	1.42	0.84
1:B:446:ARG:NH1	1:B:446:ARG:HG3	1.93	0.84
1:C:77:ARG:HH11	1:C:77:ARG:CG	1.91	0.84
1:B:318:MET:HE1	1:B:489:MET:HB2	1.58	0.84
1:C:418:ASN:HB2	1:C:422:GLN:H	1.44	0.83
1:C:77:ARG:NH1	1:C:77:ARG:HG2	1.95	0.82
1:C:375:LYS:HB3	1:C:376:LYS:HE2	1.62	0.82
1:C:412:ASN:OD1	1:C:414:GLN:HB2	1.81	0.81
1:C:101:ARG:H	1:C:120:ASN:HD21	1.27	0.81
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.45	0.80
1:C:214:THR:HG22	1:C:217:GLY:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:HH12	1:B:389:THR:HG23	1.47	0.79
1:A:419:GLU:OE1	1:A:419:GLU:HA	1.83	0.78
1:D:456:VAL:HG12	1:D:457:MET:CE	2.13	0.78
1:D:234:GLN:NE2	1:D:234:GLN:H	1.80	0.78
1:C:316:LEU:CD2	1:C:473:VAL:HG11	2.14	0.77
1:C:234:GLN:NE2	1:C:234:GLN:H	1.83	0.76
1:C:54:MET:HG3	1:C:218:GLN:HE21	1.50	0.76
1:A:456:VAL:HG12	1:A:457:MET:HE2	1.67	0.75
1:B:208:ILE:CD1	1:B:240:LEU:HB2	2.09	0.75
1:B:204:MET:O	1:B:208:ILE:HG12	1.88	0.74
1:D:407:ASN:H	1:D:415:HIS:HE1	1.36	0.74
1:C:214:THR:HG21	5:C:646:HOH:O	1.88	0.74
1:A:456:VAL:HG12	1:A:457:MET:CE	2.17	0.73
1:C:418:ASN:ND2	1:C:422:GLN:HB2	1.98	0.73
1:D:139:GLY:CA	1:D:142:LYS:HE3	2.17	0.73
1:D:234:GLN:HE21	1:D:234:GLN:H	1.35	0.73
1:B:37:PRO:HD3	1:B:61:ILE:HD13	1.70	0.73
1:A:101:ARG:CD	1:A:117:VAL:O	2.38	0.72
1:A:77:ARG:NH1	1:A:77:ARG:HG2	2.01	0.72
1:B:101:ARG:H	1:B:120:ASN:HD21	1.36	0.71
1:B:148:ARG:HD3	1:B:184:SER:HB3	1.72	0.71
1:A:32:LYS:HD2	1:A:33:LEU:H	1.55	0.71
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	1.72	0.70
1:B:346:ARG:HD2	1:B:353:GLU:OE2	1.91	0.70
1:B:446:ARG:CG	1:B:446:ARG:HH11	2.05	0.70
1:D:372:ARG:NH2	5:D:502:HOH:O	2.25	0.69
1:D:253:GLU:O	1:D:256:GLN:CB	2.41	0.69
1:C:316:LEU:HD21	1:C:473:VAL:HG11	1.75	0.68
1:D:281:ASN:ND2	1:D:283:ASN:H	1.91	0.68
1:D:352:MET:HE3	1:D:454:THR:HG22	1.75	0.68
1:C:392:TYR:HB3	1:C:394:MET:CE	2.24	0.67
1:B:318:MET:HE3	1:B:489:MET:CE	2.25	0.67
1:B:77:ARG:CG	1:B:77:ARG:HH11	2.07	0.67
1:C:61:ILE:HD11	1:C:69:PHE:CD1	2.29	0.66
1:A:420:LYS:CB	1:A:422:GLN:HE21	2.07	0.66
1:B:253:GLU:O	1:B:256:GLN:HG3	1.96	0.66
1:D:456:VAL:HG12	1:D:457:MET:HE3	1.78	0.66
1:D:139:GLY:HA2	1:D:142:LYS:HG2	1.76	0.66
1:C:234:GLN:HE21	1:C:234:GLN:N	1.85	0.66
1:C:257:ARG:HH11	1:C:257:ARG:CG	2.05	0.65
1:B:61:ILE:HD12	1:B:65:TYR:CD2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLY:O	1:D:142:LYS:HG2	1.97	0.65
1:A:101:ARG:HD3	1:A:117:VAL:O	1.94	0.65
1:A:314:PHE:HE2	1:A:457:MET:CE	2.10	0.65
1:A:30:LYS:HG3	1:A:32:LYS:H	1.62	0.64
1:B:148:ARG:HD3	1:B:184:SER:CB	2.28	0.64
1:A:420:LYS:HG3	1:A:422:GLN:NE2	2.11	0.64
1:B:233:PRO:HD2	1:B:234:GLN:NE2	2.13	0.64
1:B:200:SER:O	1:B:204:MET:HG3	1.98	0.63
1:B:318:MET:HE3	1:B:489:MET:HE3	1.80	0.63
1:C:72:HIS:NE2	1:C:77:ARG:HD3	2.14	0.63
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.79	0.63
1:B:210:GLN:HE22	1:B:476:LYS:NZ	1.97	0.63
1:A:101:ARG:HD2	1:A:117:VAL:O	1.99	0.63
1:D:50:ASN:ND2	1:D:52:GLU:H	1.96	0.62
1:D:253:GLU:O	1:D:256:GLN:HB2	2.00	0.62
1:C:418:ASN:HB2	1:C:422:GLN:N	2.15	0.61
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.34	0.61
1:C:101:ARG:CD	1:C:117:VAL:O	2.49	0.61
1:D:101:ARG:CD	1:D:117:VAL:O	2.49	0.61
1:C:352:MET:HE3	1:C:454:THR:HG22	1.83	0.61
1:A:314:PHE:CE2	1:A:457:MET:HE1	2.36	0.60
1:A:314:PHE:HE2	1:A:457:MET:HE1	1.65	0.60
1:C:324:GLU:HG3	1:C:457:MET:CE	2.31	0.60
1:A:346:ARG:HD2	1:A:353:GLU:OE1	2.00	0.60
1:C:281:ASN:ND2	1:C:283:ASN:H	1.99	0.60
1:D:101:ARG:HD2	1:D:117:VAL:O	2.02	0.60
1:B:148:ARG:HH11	1:B:184:SER:HB3	1.66	0.59
1:D:50:ASN:HD22	1:D:52:GLU:H	1.50	0.59
1:A:337:LYS:HD2	1:A:337:LYS:N	2.17	0.59
1:C:50:ASN:C	1:C:50:ASN:HD22	2.04	0.59
1:D:50:ASN:HD22	1:D:50:ASN:C	2.05	0.59
1:C:251:LYS:HZ2	1:C:251:LYS:HB3	1.67	0.59
1:B:60:LYS:HE2	5:B:958:HOH:O	2.02	0.59
1:C:251:LYS:HZ3	1:C:251:LYS:HA	1.68	0.59
1:C:45:ASN:HD22	1:C:72:HIS:N	1.93	0.59
1:A:420:LYS:CG	1:A:422:GLN:HE21	2.16	0.59
1:B:254:HIS:O	1:B:258:THR:HG22	2.03	0.59
1:C:376:LYS:HE2	1:C:376:LYS:N	2.17	0.58
1:B:253:GLU:HA	1:B:256:GLN:HG2	1.85	0.58
1:C:101:ARG:HD2	1:C:117:VAL:O	2.04	0.58
1:C:50:ASN:ND2	1:C:52:GLU:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:CD	1:A:322:GLU:H	2.01	0.58
1:C:352:MET:CE	1:C:454:THR:HG22	2.34	0.58
1:B:101:ARG:CD	1:B:117:VAL:O	2.51	0.58
1:B:318:MET:CE	1:B:489:MET:HB2	2.30	0.58
1:B:64:ARG:NH1	5:B:1038:HOH:O	2.37	0.58
1:D:232:GLY:HA3	1:D:234:GLN:HE22	1.69	0.58
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.39	0.57
1:D:186:VAL:CG1	1:D:295:THR:HG23	2.34	0.57
1:C:32:LYS:HE2	1:C:384:PHE:HB2	1.85	0.57
1:B:208:ILE:HD13	1:B:240:LEU:HD12	1.85	0.57
1:D:142:LYS:O	1:D:144:GLY:N	2.38	0.57
1:A:476:LYS:HE2	1:A:477:HIS:NE2	2.20	0.57
1:C:186:VAL:CG1	1:C:295:THR:HG23	2.35	0.57
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.41	0.56
1:B:337:LYS:NZ	1:B:496:HIS:CE1	2.73	0.56
1:C:473:VAL:HG12	1:C:473:VAL:O	2.05	0.56
1:A:205:MET:O	1:A:208:ILE:HG12	2.05	0.56
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.88	0.56
1:D:376:LYS:HA	1:D:387:LYS:HB2	1.88	0.56
1:B:101:ARG:HD3	1:B:117:VAL:O	2.06	0.55
1:A:117:VAL:CG1	1:A:370[A]:LEU:HD21	2.37	0.54
1:B:210:GLN:O	1:B:214:THR:HG23	2.07	0.54
1:C:117:VAL:HG22	2:C:500:HEM:HAD1	1.88	0.54
1:A:353:GLU:HG2	1:A:423:PHE:CD2	2.43	0.54
1:C:37:PRO:HD3	1:C:61:ILE:HD13	1.89	0.54
1:C:281:ASN:HD22	1:C:282:PRO:N	2.06	0.54
1:D:281:ASN:HD22	1:D:281:ASN:C	2.10	0.54
1:C:95:ALA:HB1	1:C:436:LYS:HD3	1.90	0.53
1:A:420:LYS:CG	1:A:422:GLN:NE2	2.70	0.53
1:D:76:ARG:NH2	1:D:103:GLU:HG3	2.24	0.53
1:D:418:ASN:HB2	1:D:422:GLN:H	1.73	0.53
1:C:250:LYS:HD2	5:C:665:HOH:O	2.08	0.53
1:B:253:GLU:HA	1:B:256:GLN:CG	2.39	0.53
1:B:337:LYS:HZ2	1:B:496:HIS:CE1	2.26	0.53
1:B:419:GLU:CD	1:B:419:GLU:H	2.11	0.53
1:D:186:VAL:HG11	1:D:295:THR:HG23	1.90	0.53
1:A:342:LYS:HE3	1:A:344:GLU:OE1	2.08	0.52
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.91	0.52
1:B:271:PHE:CE2	1:B:291:LEU:HB2	2.44	0.52
1:C:354:ALA:HB2	1:C:417:LEU:HD13	1.91	0.52
1:C:101:ARG:HD3	1:C:117:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:HIS:NE2	1:A:77:ARG:HD3	2.24	0.52
1:C:77:ARG:NH1	5:C:647:HOH:O	2.07	0.52
1:B:450:PHE:O	1:B:454:THR:HG23	2.10	0.52
1:C:205:MET:HE2	1:C:300:ILE:HG12	1.92	0.52
1:C:375:LYS:HB3	1:C:376:LYS:CE	2.38	0.52
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.75	0.52
1:D:420:LYS:HB2	1:D:422:GLN:HE21	1.74	0.52
1:D:476:LYS:HB2	1:D:485:ARG:HA	1.90	0.52
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.69	0.51
1:D:466:GLN:HG3	1:D:471:ILE:CG1	2.40	0.51
1:B:33:LEU:HD21	1:B:77:ARG:HD2	1.91	0.51
1:C:50:ASN:HD22	1:C:52:GLU:H	1.57	0.51
1:B:463:LYS:HB3	1:B:490:SER:HB2	1.93	0.51
1:B:258:THR:HG23	1:B:265:ARG:HH22	1.75	0.51
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.93	0.51
1:D:281:ASN:C	1:D:281:ASN:ND2	2.64	0.51
1:C:251:LYS:NZ	1:C:251:LYS:HB3	2.24	0.51
1:A:281:ASN:ND2	1:A:283:ASN:H	2.08	0.51
1:C:253:GLU:HA	1:C:256:GLN:HE21	1.76	0.51
1:D:407:ASN:H	1:D:415:HIS:CE1	2.23	0.50
1:C:346:ARG:HG2	1:C:353:GLU:OE1	2.11	0.50
1:D:253:GLU:O	1:D:256:GLN:HB3	2.11	0.50
1:D:129:ARG:HD2	5:D:562:HOH:O	2.12	0.50
1:B:318:MET:HE3	1:B:489:MET:HE2	1.93	0.50
1:C:418:ASN:HB3	1:C:420:LYS:H	1.76	0.50
1:D:418:ASN:HB3	1:D:420:LYS:H	1.76	0.50
1:B:61:ILE:HD12	1:B:65:TYR:HD2	1.76	0.50
1:C:369:SER:HB2	1:C:395:LEU:HG	1.92	0.50
1:B:62:SER:HB3	1:B:69:PHE:CE2	2.47	0.50
1:D:142:LYS:HG3	1:D:144:GLY:H	1.77	0.50
1:D:457:MET:HE1	1:D:462:LEU:HD21	1.93	0.50
1:A:143:ARG:O	1:A:147:GLU:HG2	2.13	0.49
1:B:61:ILE:HD11	1:B:69:PHE:CD1	2.47	0.49
1:C:72:HIS:HE2	1:C:77:ARG:HD3	1.77	0.49
1:D:466:GLN:HG3	1:D:471:ILE:HG13	1.93	0.49
1:B:352:MET:CE	1:B:454:THR:HG22	2.37	0.49
1:C:476:LYS:HB2	1:C:485:ARG:HA	1.95	0.49
1:D:281:ASN:HD22	1:D:282:PRO:HD2	1.77	0.49
1:A:302:GLY:HA2	2:A:500:HEM:HMC2	1.94	0.49
1:C:281:ASN:C	1:C:281:ASN:HD22	2.15	0.49
1:D:244:LEU:HB3	1:D:296:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:MET:HE2	1:D:300:ILE:HA	1.95	0.49
1:A:186:VAL:HA	1:A:267:PHE:HB3	1.95	0.48
1:B:271:PHE:HB3	1:B:291:LEU:HD13	1.94	0.48
1:C:281:ASN:HD22	1:C:282:PRO:CD	2.25	0.48
1:C:316:LEU:HD23	1:C:473:VAL:HG11	1.91	0.48
1:C:186:VAL:HG13	1:C:295:THR:HG23	1.94	0.48
1:C:251:LYS:NZ	1:C:251:LYS:CB	2.77	0.48
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.44	0.48
1:D:418:ASN:HD22	1:D:422:GLN:NE2	2.11	0.48
1:A:89:GLU:O	1:A:93:ASP:HB2	2.14	0.47
1:B:101:ARG:N	1:B:120:ASN:HD21	2.07	0.47
1:B:32:LYS:HE2	1:B:379:LYS:NZ	2.29	0.47
1:C:463:LYS:HB3	1:C:490:SER:HB2	1.96	0.47
1:B:103:GLU:HB2	1:B:108:ASP:OD2	2.14	0.47
1:B:120:ASN:OD1	1:B:375:LYS:HE2	2.14	0.47
1:D:400:ARG:CZ	5:D:569:HOH:O	2.63	0.47
1:C:101:ARG:N	1:C:120:ASN:HD21	2.04	0.47
1:C:392:TYR:HB3	1:C:394:MET:HE3	1.94	0.47
1:C:76:ARG:NH2	1:C:103:GLU:HG3	2.30	0.47
1:A:30:LYS:HG3	1:A:31:GLY:N	2.30	0.47
1:C:205:MET:HE2	1:C:300:ILE:HA	1.96	0.47
1:A:50:ASN:ND2	1:A:52:GLU:H	2.13	0.47
1:B:494:ARG:O	1:B:495:HIS:HB2	2.14	0.46
1:B:101:ARG:HD2	1:B:117:VAL:O	2.15	0.46
1:B:369:SER:HB2	1:B:395:LEU:HG	1.97	0.46
1:B:210:GLN:HE22	1:B:476:LYS:HZ1	1.62	0.46
1:C:205:MET:HE2	1:C:300:ILE:CG1	2.46	0.46
1:D:143:ARG:O	1:D:147:GLU:HG3	2.15	0.46
1:B:233:PRO:HD2	1:B:234:GLN:HE22	1.78	0.46
1:B:324:GLU:HG3	1:B:457:MET:CE	2.46	0.46
4:B:900:GOL:HO1	4:B:900:GOL:C1	2.14	0.46
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.97	0.46
1:C:251:LYS:CA	1:C:251:LYS:HZ3	2.28	0.46
1:C:312:TYR:HE2	1:C:473:VAL:CG1	2.29	0.46
1:B:318:MET:SD	1:B:464:SER:HB3	2.56	0.46
1:C:125:LYS:NZ	5:C:698:HOH:O	2.48	0.46
1:D:139:GLY:N	1:D:142:LYS:HE3	2.31	0.46
1:D:76:ARG:CZ	1:D:103:GLU:HG3	2.45	0.46
1:A:215:SER:CB	1:B:233:PRO:HG3	2.46	0.45
1:B:259:LEU:O	1:B:261:PRO:HD3	2.15	0.45
1:B:77:ARG:NH1	1:B:389:THR:HG23	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ARG:HD3	1:D:117:VAL:O	2.15	0.45
1:B:271:PHE:CG	1:B:291:LEU:HD13	2.51	0.45
1:D:115:GLY:O	1:D:119:SER:HB3	2.15	0.45
1:C:77:ARG:NH1	1:C:77:ARG:CG	2.61	0.45
1:D:331:ILE:HD11	1:D:352:MET:CE	2.47	0.45
1:C:312:TYR:HE2	1:C:473:VAL:HG12	1.81	0.45
1:A:135:LEU:HD12	1:A:185:ILE:HG21	1.98	0.45
1:A:357:HIS:NE2	1:A:446:ARG:NH2	2.65	0.45
1:D:432:PHE:HB3	1:D:439:CYS:HB3	1.99	0.45
1:A:50:ASN:C	1:A:50:ASN:HD22	2.20	0.45
1:A:302:GLY:HA2	2:A:500:HEM:CMC	2.47	0.45
1:B:74:GLY:N	1:B:222:MET:HE3	2.32	0.45
1:B:433:SER:HB3	2:B:500:HEM:HBA1	1.99	0.45
1:C:324:GLU:HG3	1:C:457:MET:HE1	1.99	0.45
1:D:457:MET:CE	1:D:462:LEU:HD21	2.47	0.45
1:D:60:LYS:HE2	5:D:611:HOH:O	2.16	0.45
1:B:168:ILE:O	1:B:488:THR:HA	2.17	0.44
1:C:52:GLU:HG2	1:C:52:GLU:O	2.17	0.44
1:A:281:ASN:HD22	1:A:281:ASN:C	2.20	0.44
1:D:433:SER:HB3	2:D:500:HEM:HBA1	1.98	0.44
1:B:453:PHE:O	1:B:457:MET:HG2	2.17	0.44
1:D:236:GLN:O	1:D:240:LEU:HG	2.18	0.44
1:C:186:VAL:HA	1:C:267:PHE:HB3	2.00	0.44
1:C:61:ILE:HD12	1:C:61:ILE:O	2.18	0.44
1:A:33:LEU:HD12	1:A:384:PHE:O	2.17	0.44
1:B:264:PRO:HG3	1:B:273:ILE:CD1	2.48	0.44
1:B:370:LEU:HA	4:B:900:GOL:H12	1.99	0.44
1:D:367:PRO:HD2	1:D:480:PHE:O	2.18	0.44
1:C:61:ILE:HD12	1:C:65:TYR:HD2	1.83	0.44
1:C:418:ASN:HB3	1:C:420:LYS:N	2.33	0.43
1:C:97:GLU:HG3	5:C:705:HOH:O	2.18	0.43
1:A:125:LYS:HD2	5:A:556:HOH:O	2.18	0.43
1:C:210:GLN:NE2	1:C:476:LYS:NZ	2.66	0.43
1:A:77:ARG:NH1	1:A:77:ARG:CG	2.75	0.43
1:A:423:PHE:HE1	1:A:425:LYS:HG2	1.83	0.43
1:C:259:LEU:HG	1:C:260:ASP:N	2.32	0.43
1:D:450:PHE:O	1:D:454:THR:HG23	2.18	0.43
1:A:375:LYS:HA	1:A:375:LYS:HD2	1.85	0.43
1:A:314:PHE:HE2	1:A:457:MET:HE3	1.83	0.43
1:A:101:ARG:NH2	1:A:370[A]:LEU:HB3	2.33	0.43
1:A:92:VAL:HG23	1:A:434:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ALA:O	1:A:157:ILE:HG12	2.19	0.43
1:A:176:ARG:NE	5:A:627:HOH:O	2.32	0.43
1:B:145:ILE:HA	1:B:145:ILE:HD12	1.71	0.43
1:B:37:PRO:HD3	1:B:61:ILE:CD1	2.45	0.43
1:C:76:ARG:CZ	1:C:103:GLU:HG3	2.48	0.43
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.68	0.43
1:C:257:ARG:NH1	1:C:257:ARG:CG	2.72	0.43
1:C:271:PHE:CD2	1:C:291:LEU:HB2	2.54	0.43
1:C:33:LEU:HD12	1:C:384:PHE:O	2.19	0.43
1:B:281:ASN:C	1:B:281:ASN:HD22	2.22	0.42
1:B:46:TYR:HA	1:B:222:MET:HE1	2.01	0.42
1:D:260:ASP:O	1:D:262:ASN:N	2.52	0.42
1:A:126:GLN:HG2	5:A:594:HOH:O	2.19	0.42
1:A:354:ALA:HB2	1:A:417:LEU:HD13	2.01	0.42
1:B:143:ARG:O	1:B:147:GLU:HG3	2.19	0.42
1:D:365:VAL:O	1:D:481:ALA:HA	2.20	0.42
1:A:281:ASN:HD22	1:A:282:PRO:CD	2.32	0.42
1:B:271:PHE:CB	1:B:291:LEU:HD13	2.50	0.42
1:B:377:ASP:HB3	1:B:384:PHE:CZ	2.55	0.42
1:C:143:ARG:NE	1:C:147:GLU:HG3	2.34	0.42
1:C:152:GLU:HG3	1:C:177:THR:HG23	2.01	0.42
1:C:450:PHE:O	1:C:454:THR:HG23	2.19	0.42
1:A:32:LYS:HG3	1:A:33:LEU:O	2.19	0.42
1:B:380:PHE:O	1:B:383:PHE:HB2	2.20	0.41
1:A:442:GLU:O	1:A:446:ARG:HG3	2.21	0.41
1:B:74:GLY:H	1:B:222:MET:HE3	1.85	0.41
1:B:210:GLN:NE2	1:B:476:LYS:NZ	2.67	0.41
1:A:339:ARG:CZ	1:A:342:LYS:HZ1	2.34	0.41
1:B:195:ASP:C	1:B:195:ASP:OD1	2.58	0.41
1:B:412:ASN:OD1	1:B:414:GLN:HB2	2.21	0.41
1:A:381:ARG:O	1:A:382:ASP:HB2	2.21	0.41
1:C:148:ARG:HD3	1:C:184:SER:OG	2.20	0.41
1:D:354:ALA:HB2	1:D:417:LEU:HD13	2.02	0.41
1:A:50:ASN:C	1:A:50:ASN:ND2	2.74	0.41
1:C:211:PHE:O	1:C:214:THR:HB	2.21	0.41
1:A:346:ARG:HE	1:A:346:ARG:HB3	1.55	0.41
1:A:476:LYS:HB2	1:A:485:ARG:HA	2.03	0.41
1:B:32:LYS:HE2	1:B:379:LYS:HZ2	1.86	0.41
1:A:148:ARG:HD3	1:A:184:SER:OG	2.21	0.40
1:B:172:PHE:O	1:B:176:ARG:HG3	2.20	0.40
1:C:352:MET:HG2	1:C:454:THR:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:SER:O	1:D:204:MET:HG3	2.21	0.40
1:B:57:SER:O	1:B:61:ILE:HG23	2.21	0.40
1:B:463:LYS:HD2	1:B:463:LYS:HA	1.79	0.40
1:B:54:MET:HG3	1:B:218:GLN:NE2	2.23	0.40
1:C:103:GLU:HG2	1:C:390:GLU:OE2	2.22	0.40
1:D:174:LEU:HA	1:D:174:LEU:HD12	1.91	0.40
1:D:342:LYS:HB2	1:D:342:LYS:HE3	1.71	0.40
1:A:95:ALA:HB1	1:A:436:LYS:HG2	2.04	0.40
1:B:180:ASN:HA	1:B:183:SER:HB2	2.02	0.40
1:C:176:ARG:HE	1:C:176:ARG:HB2	1.73	0.40
1:C:246:ASP:O	1:C:250:LYS:HG3	2.21	0.40
1:A:168:ILE:O	1:A:488:THR:HA	2.22	0.40
1:A:369:SER:HB2	1:A:395:LEU:HG	2.03	0.40
1:B:247:PHE:CZ	1:B:251:LYS:HE3	2.55	0.40
1:B:258:THR:O	1:B:258:THR:OG1	2.37	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	464/476 (98%)	453 (98%)	11 (2%)	0	100	100
1	B	463/476 (97%)	445 (96%)	16 (4%)	2 (0%)	38	26
1	C	462/476 (97%)	447 (97%)	15 (3%)	0	100	100
1	D	462/476 (97%)	447 (97%)	13 (3%)	2 (0%)	38	26
All	All	1851/1904 (97%)	1792 (97%)	55 (3%)	4 (0%)	51	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	495	HIS
1	D	143	ARG
1	B	261	PRO
1	D	261	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	413/422 (98%)	397 (96%)	16 (4%)	37	26
1	B	413/422 (98%)	393 (95%)	20 (5%)	30	18
1	C	411/422 (97%)	390 (95%)	21 (5%)	28	16
1	D	411/422 (97%)	390 (95%)	21 (5%)	28	16
All	All	1648/1688 (98%)	1570 (95%)	78 (5%)	30	19

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	77	ARG
1	A	101	ARG
1	A	135	LEU
1	A	167	ASN
1	A	210	GLN
1	A	236	GLN
1	A	281	ASN
1	A	312	TYR
1	A	316	LEU
1	A	353	GLU
1	A	373	ARG
1	A	417	LEU
1	A	419	GLU
1	A	465	SER
1	A	468	PRO
1	B	61	ILE
1	B	135	LEU

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Mol	Chain	Res	Type
1	B	143	ARG
1	B	167	ASN
1	B	174	LEU
1	B	210	GLN
1	B	234	GLN
1	B	256	GLN
1	B	260	ASP
1	B	261	PRO
1	B	280	LYS
1	B	281	ASN
1	B	312	TYR
1	B	316	LEU
1	B	414	GLN
1	B	417	LEU
1	B	419	GLU
1	B	446	ARG
1	B	463	LYS
1	B	468	PRO
1	C	50	ASN
1	C	61	ILE
1	C	77	ARG
1	C	101	ARG
1	C	126	GLN
1	C	135	LEU
1	C	143	ARG
1	C	148	ARG
1	C	174	LEU
1	C	214	THR
1	C	234	GLN
1	C	257	ARG
1	C	274	ARG
1	C	281	ASN
1	C	312	TYR
1	C	340	GLN
1	C	344	GLU
1	C	376	LYS
1	C	414	GLN
1	C	417	LEU
1	C	467	SER
1	D	39	PRO
1	D	40	LEU
1	D	50	ASN

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Mol	Chain	Res	Type
1	D	101	ARG
1	D	135	LEU
1	D	174	LEU
1	D	210	GLN
1	D	234	GLN
1	D	258	THR
1	D	279	GLU
1	D	281	ASN
1	D	312	TYR
1	D	316	LEU
1	D	337	LYS
1	D	353	GLU
1	D	375	LYS
1	D	417	LEU
1	D	419	GLU
1	D	465	SER
1	D	469	LYS
1	D	473	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	53	GLN
1	A	56	ASN
1	A	210	GLN
1	A	218	GLN
1	A	276	GLN
1	A	281	ASN
1	A	283	ASN
1	A	422	GLN
1	B	48	GLN
1	B	50	ASN
1	B	56	ASN
1	B	94	GLN
1	B	210	GLN
1	B	218	GLN
1	B	234	GLN
1	B	236	GLN
1	B	281	ASN
1	B	328	HIS
1	B	340	GLN

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Mol	Chain	Res	Type
1	B	477	HIS
1	C	45	ASN
1	C	50	ASN
1	C	53	GLN
1	C	56	ASN
1	C	94	GLN
1	C	120	ASN
1	C	126	GLN
1	C	167	ASN
1	C	210	GLN
1	C	218	GLN
1	C	234	GLN
1	C	256	GLN
1	C	281	ASN
1	C	328	HIS
1	C	418	ASN
1	C	422	GLN
1	D	50	ASN
1	D	53	GLN
1	D	56	ASN
1	D	94	GLN
1	D	210	GLN
1	D	218	GLN
1	D	234	GLN
1	D	239	GLN
1	D	256	GLN
1	D	262	ASN
1	D	281	ASN
1	D	283	ASN
1	D	415	HIS
1	D	418	ASN
1	D	422	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

9 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	HEM	A	500	1	28,50,50	1.87	8 (28%)	17,82,82	1.21	2 (11%)
3	COU	A	501	-	10,12,12	1.99	4 (40%)	10,16,16	1.14	1 (10%)
2	HEM	B	500	1	28,50,50	2.11	12 (42%)	17,82,82	1.41	2 (11%)
3	COU	B	501	-	10,12,12	2.19	5 (50%)	10,16,16	1.15	1 (10%)
4	GOL	B	900	-	5,5,5	5.13	3 (60%)	5,5,5	5.67	3 (60%)
2	HEM	C	500	1	28,50,50	2.36	10 (35%)	17,82,82	1.73	4 (23%)
3	COU	C	501	-	10,12,12	1.74	3 (30%)	10,16,16	0.97	1 (10%)
2	HEM	D	500	1	28,50,50	2.00	9 (32%)	17,82,82	1.58	4 (23%)
3	COU	D	501	-	10,12,12	2.26	5 (50%)	10,16,16	1.23	1 (10%)

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	HEM	A	500	1	-	0/6/54/54	0/0/8/8
3	COU	A	501	-	-	0/0/0/0	0/2/2/2
2	HEM	B	500	1	-	0/6/54/54	0/0/8/8
3	COU	B	501	-	-	0/0/0/0	0/2/2/2
4	GOL	B	900	-	-	0/4/4/4	0/0/0/0
2	HEM	C	500	1	-	0/6/54/54	0/0/8/8
3	COU	C	501	-	-	0/0/0/0	0/2/2/2
2	HEM	D	500	1	-	0/6/54/54	0/0/8/8
3	COU	D	501	-	-	0/0/0/0	0/2/2/2

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	900	GOL	C3-C2	-8.43	1.21	1.52
2	C	500	HEM	C1C-NC	-7.03	1.28	1.36
2	C	500	HEM	C3C-CAC	-4.97	1.37	1.47
2	A	500	HEM	C3C-CAC	-4.95	1.37	1.47
2	D	500	HEM	C3C-CAC	-4.90	1.38	1.47
2	B	500	HEM	C3C-CAC	-4.39	1.39	1.47
2	B	500	HEM	C4D-ND	-4.32	1.31	1.36
2	D	500	HEM	C1B-NB	-2.96	1.33	1.36
2	C	500	HEM	C4C-NC	-2.81	1.33	1.36
2	D	500	HEM	C1C-NC	-2.71	1.33	1.36
2	B	500	HEM	C4A-NA	-2.69	1.30	1.36
2	B	500	HEM	C4C-NC	-2.68	1.33	1.36
2	D	500	HEM	C4A-NA	-2.67	1.30	1.36
2	A	500	HEM	C4D-ND	-2.65	1.33	1.36
2	C	500	HEM	C3B-CAB	-2.51	1.42	1.47
2	B	500	HEM	C1D-ND	-2.49	1.30	1.36
2	D	500	HEM	C4D-ND	-2.46	1.33	1.36
2	A	500	HEM	C3C-C2C	-2.45	1.37	1.40
2	A	500	HEM	C1C-NC	-2.31	1.34	1.36
2	C	500	HEM	C4D-ND	-2.30	1.34	1.36
2	B	500	HEM	C1C-NC	-2.25	1.34	1.36
2	D	500	HEM	C4C-NC	-2.18	1.34	1.36
2	A	500	HEM	C1D-ND	-2.16	1.31	1.36
2	C	500	HEM	C1D-ND	-2.12	1.31	1.36
2	B	500	HEM	C1D-CHD	-2.08	1.34	1.40
2	C	500	HEM	CMD-C2D	2.05	1.55	1.51
3	A	501	COU	C7-C8	2.07	1.41	1.36
3	C	501	COU	C3-C4	2.09	1.47	1.41
2	B	500	HEM	CMD-C2D	2.16	1.56	1.51
3	C	501	COU	O2-C9	2.19	1.40	1.36
3	D	501	COU	C3-C4	2.25	1.47	1.41
3	B	501	COU	C7-C6	2.30	1.43	1.38
3	A	501	COU	C7-C6	2.30	1.43	1.38
3	D	501	COU	C7-C6	2.39	1.43	1.38
3	D	501	COU	C7-C8	2.40	1.42	1.36
3	B	501	COU	C3-C4	2.45	1.47	1.41
2	A	500	HEM	CBB-CAB	2.53	1.46	1.28
3	B	501	COU	C7-C8	2.58	1.42	1.36
2	D	500	HEM	CBB-CAB	2.58	1.47	1.28
2	C	500	HEM	CBB-CAB	2.59	1.47	1.28
2	B	500	HEM	CMA-C3A	2.60	1.56	1.51
2	B	500	HEM	CBB-CAB	2.81	1.48	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	CMD-C2D	2.95	1.57	1.51
3	B	501	COU	O2-C9	3.03	1.41	1.36
2	C	500	HEM	C3B-C2B	3.06	1.44	1.40
3	A	501	COU	O2-C9	3.07	1.41	1.36
4	B	900	GOL	O3-C3	3.09	1.55	1.42
2	B	500	HEM	CMB-C2B	3.28	1.58	1.51
2	D	500	HEM	CMA-C3A	3.37	1.58	1.51
3	C	501	COU	C2-C1	3.41	1.44	1.37
2	B	500	HEM	C3B-C2B	3.46	1.44	1.40
2	D	500	HEM	CMD-C2D	3.48	1.58	1.51
3	D	501	COU	O2-C9	3.78	1.42	1.36
3	A	501	COU	C2-C1	3.88	1.45	1.37
3	D	501	COU	C2-C1	3.93	1.45	1.37
3	B	501	COU	C2-C1	4.11	1.45	1.37
2	C	500	HEM	CMA-C3A	4.14	1.60	1.51
2	A	500	HEM	CMA-C3A	4.51	1.60	1.51
4	B	900	GOL	O1-C1	6.86	1.71	1.42

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	HEM	C4C-C3C-C2C	-4.22	103.95	106.90
2	D	500	HEM	C4C-C3C-C2C	-2.72	105.00	106.90
2	B	500	HEM	C4C-C3C-C2C	-2.68	105.03	106.90
3	C	501	COU	C3-C2-C1	2.00	121.00	118.45
2	A	500	HEM	CAD-CBD-CGD	2.01	116.10	112.66
3	A	501	COU	C3-C2-C1	2.16	121.20	118.45
2	C	500	HEM	CAD-CBD-CGD	2.17	116.36	112.66
2	D	500	HEM	CMC-C2C-C3C	2.24	129.05	124.89
3	B	501	COU	C3-C2-C1	2.36	121.45	118.45
3	D	501	COU	C3-C2-C1	2.68	121.87	118.45
2	A	500	HEM	CAA-CBA-CGA	2.72	117.31	112.66
2	D	500	HEM	CMB-C2B-C3B	2.78	130.05	124.89
2	C	500	HEM	CMB-C2B-C3B	2.79	130.07	124.89
2	C	500	HEM	CAA-CBA-CGA	2.87	117.57	112.66
2	D	500	HEM	CAA-CBA-CGA	2.93	117.67	112.66
2	B	500	HEM	CMB-C2B-C3B	3.45	131.30	124.89
4	B	900	GOL	O1-C1-C2	3.92	129.80	110.07
4	B	900	GOL	O2-C2-C3	5.52	134.89	108.84
4	B	900	GOL	O3-C3-C2	10.62	163.59	110.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	4	0
2	B	500	HEM	1	0
4	B	900	GOL	3	0
2	C	500	HEM	1	0
2	D	500	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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	465/476 (97%)	0.09	10 (2%) 62 66	26, 38, 57, 80	0
1	B	465/476 (97%)	0.28	7 (1%) 74 77	30, 44, 63, 92	0
1	C	464/476 (97%)	-0.16	1 (0%) 94 95	26, 38, 56, 71	0
1	D	464/476 (97%)	-0.03	8 (1%) 70 73	26, 39, 66, 79	0
All	All	1858/1904 (97%)	0.05	26 (1%) 75 78	26, 40, 61, 92	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	GLY	7.2
1	B	496	HIS	7.0
1	D	143	ARG	5.1
1	A	30	LYS	4.7
1	B	495	HIS	4.5
1	D	31	GLY	4.1
1	D	280	LYS	3.7
1	A	206	LEU	2.9
1	A	300	ILE	2.8
1	A	210	GLN	2.7
1	D	138	PHE	2.6
1	B	257	ARG	2.6
1	A	208	ILE	2.6
1	B	382	ASP	2.5
1	B	61	ILE	2.5
1	D	142	LYS	2.5
1	B	143	ARG	2.5
1	A	207	GLY	2.4
1	A	408	PRO	2.2
1	B	405	PHE	2.2
1	D	141	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	420	LYS	2.1
1	A	419	GLU	2.1
1	A	273	ILE	2.1
1	A	209	PHE	2.0
1	D	196	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	GOL	B	900	6/6	0.78	0.35	8.48	37,43,43,46	0
3	COU	D	501	11/11	0.86	0.18	6.03	50,56,57,57	0
3	COU	C	501	11/11	0.91	0.19	4.68	59,61,62,62	0
3	COU	A	501	11/11	0.92	0.20	1.35	56,59,60,60	0
3	COU	B	501	11/11	0.93	0.16	0.66	63,64,64,65	0
2	HEM	C	500	43/43	0.99	0.11	0.42	26,32,34,36	0
2	HEM	A	500	43/43	0.99	0.13	0.29	24,28,34,37	0
2	HEM	B	500	43/43	0.99	0.12	0.10	28,33,39,42	0
2	HEM	D	500	43/43	0.99	0.12	0.09	27,31,34,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.