



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:07 pm GMT

PDB ID : 4XRZ  
Title : Human Cytochrome P450 2D6 BACE1 Inhibitor 6 Complex  
Authors : Johnson, E.F.; Fan, Y.  
Deposited on : 2015-01-21  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

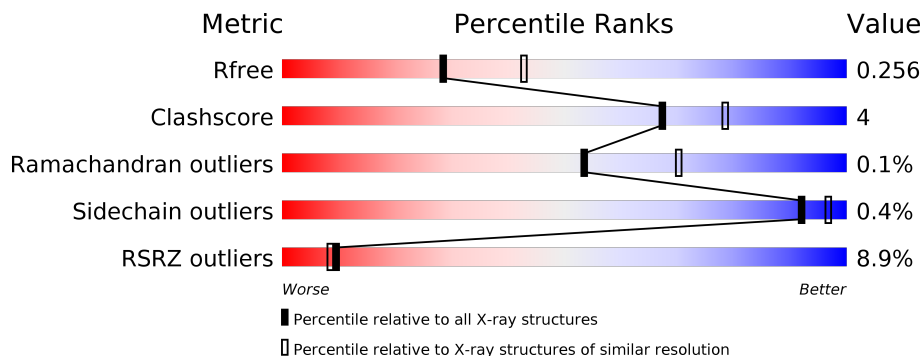
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	111664	3481 (2.40-2.40)
Clashscore	122126	3956 (2.40-2.40)
Ramachandran outliers	120053	3897 (2.40-2.40)
Sidechain outliers	120020	3898 (2.40-2.40)
RSRZ outliers	108989	3386 (2.40-2.40)

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	479	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>5%</div> </div> </div>
1	B	479	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>•</div> </div> </div>
1	C	479	<div> <div>10%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
1	D	479	<div> <div>9%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15092 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 2D6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	0	0
			3618	2319	641	644	14			
1	B	458	Total	C	N	O	S	0	0	0
			3625	2324	642	645	14			
1	C	455	Total	C	N	O	S	0	0	0
			3599	2306	639	640	14			
1	D	455	Total	C	N	O	S	0	0	0
			3599	2306	639	640	14			

There are 60 discrepancies between the modelled and reference sequences:

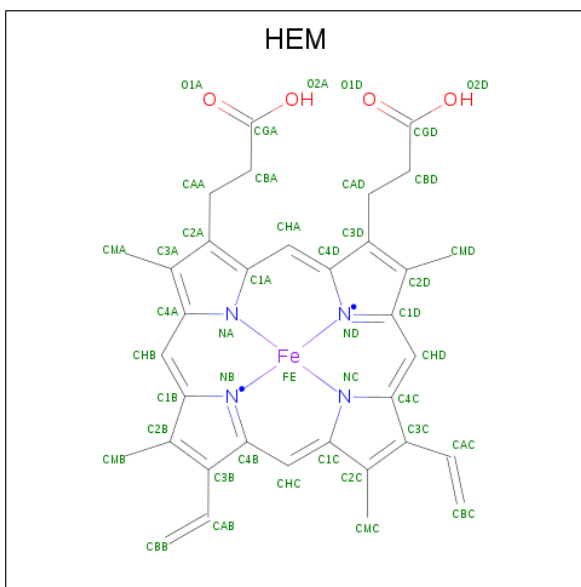
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP P10635
A	24	ALA	-	expression tag	UNP P10635
A	25	LYS	-	expression tag	UNP P10635
A	26	LYS	-	expression tag	UNP P10635
A	27	THR	-	expression tag	UNP P10635
A	28	SER	-	expression tag	UNP P10635
A	29	SER	-	expression tag	UNP P10635
A	30	LYS	-	expression tag	UNP P10635
A	31	GLY	-	expression tag	UNP P10635
A	32	LYS	-	expression tag	UNP P10635
A	33	LEU	-	expression tag	UNP P10635
A	498	HIS	-	expression tag	UNP P10635
A	499	HIS	-	expression tag	UNP P10635
A	500	HIS	-	expression tag	UNP P10635
A	501	HIS	-	expression tag	UNP P10635
B	23	MET	-	expression tag	UNP P10635
B	24	ALA	-	expression tag	UNP P10635
B	25	LYS	-	expression tag	UNP P10635
B	26	LYS	-	expression tag	UNP P10635
B	27	THR	-	expression tag	UNP P10635
B	28	SER	-	expression tag	UNP P10635

*Continued on next page...*

*Continued from previous page...*

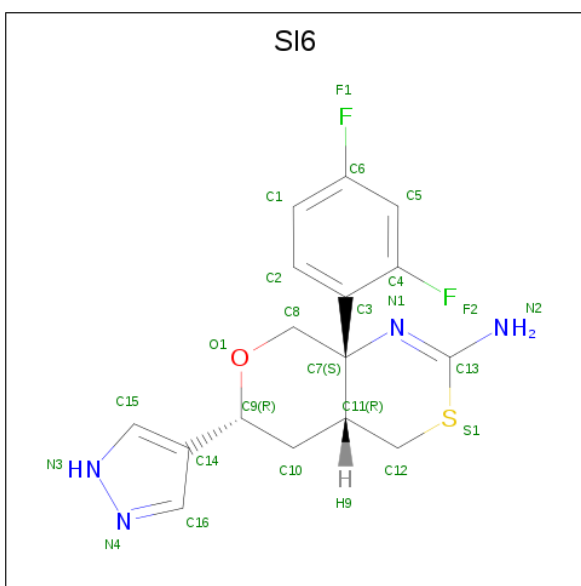
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP P10635
B	500	HIS	-	expression tag	UNP P10635
B	501	HIS	-	expression tag	UNP P10635
C	23	MET	-	expression tag	UNP P10635
C	24	ALA	-	expression tag	UNP P10635
C	25	LYS	-	expression tag	UNP P10635
C	26	LYS	-	expression tag	UNP P10635
C	27	THR	-	expression tag	UNP P10635
C	28	SER	-	expression tag	UNP P10635
C	29	SER	-	expression tag	UNP P10635
C	30	LYS	-	expression tag	UNP P10635
C	31	GLY	-	expression tag	UNP P10635
C	32	LYS	-	expression tag	UNP P10635
C	33	LEU	-	expression tag	UNP P10635
C	498	HIS	-	expression tag	UNP P10635
C	499	HIS	-	expression tag	UNP P10635
C	500	HIS	-	expression tag	UNP P10635
C	501	HIS	-	expression tag	UNP P10635
D	23	MET	-	expression tag	UNP P10635
D	24	ALA	-	expression tag	UNP P10635
D	25	LYS	-	expression tag	UNP P10635
D	26	LYS	-	expression tag	UNP P10635
D	27	THR	-	expression tag	UNP P10635
D	28	SER	-	expression tag	UNP P10635
D	29	SER	-	expression tag	UNP P10635
D	30	LYS	-	expression tag	UNP P10635
D	31	GLY	-	expression tag	UNP P10635
D	32	LYS	-	expression tag	UNP P10635
D	33	LEU	-	expression tag	UNP P10635
D	498	HIS	-	expression tag	UNP P10635
D	499	HIS	-	expression tag	UNP P10635
D	500	HIS	-	expression tag	UNP P10635
D	501	HIS	-	expression tag	UNP P10635

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 3 is (4aR,6R,8aS)-8a-(2,4-difluorophenyl)-6-(1H-pyrazol-4-yl)-4,4a,5,6,8,8a-hexahydrodropyrano[3,4-d][1,3]thiazin-2-amine (three-letter code: SI6) (formula: C<sub>16</sub>H<sub>16</sub>F<sub>2</sub>N<sub>4</sub>OS).

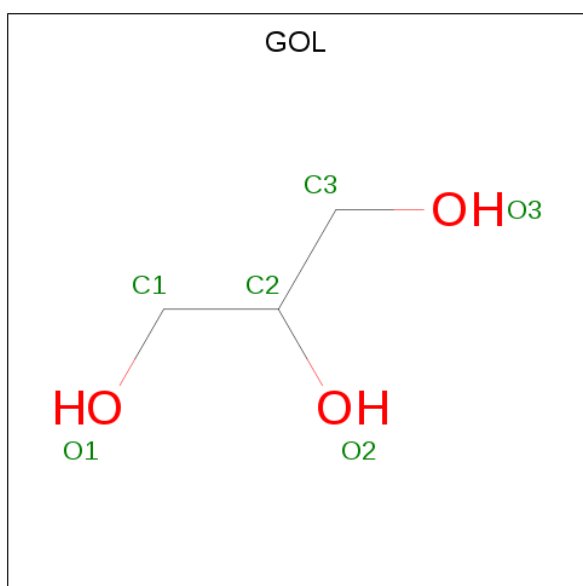


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			24	16	2	4	1	1		
3	B	1	Total	C	F	N	O	S	0	0
			24	16	2	4	1	1		
3	C	1	Total	C	F	N	O	S	0	0
			24	16	2	4	1	1		
3	D	1	Total	C	F	N	O	S	0	0
			24	16	2	4	1	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	A	4	Total	Zn	0	0
			4	4		
4	D	3	Total	Zn	0	0
			3	3		
4	C	3	Total	Zn	0	0
			3	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Na	0	0
			1	1		
6	A	1	Total	Na	0	0
			1	1		
6	D	1	Total	Na	0	0
			1	1		
6	C	1	Total	Na	0	0
			1	1		

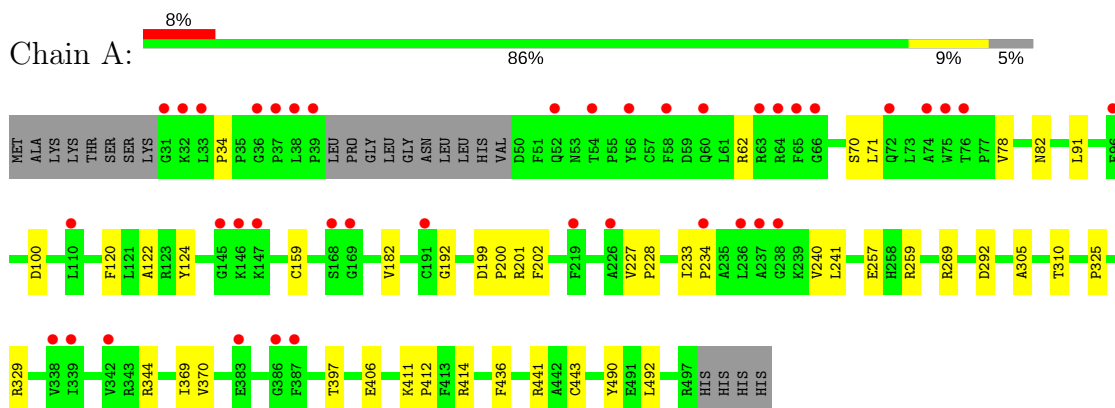
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	91	Total	O	0	0
			91	91		
7	B	97	Total	O	0	0
			97	97		
7	C	73	Total	O	0	0
			73	73		
7	D	82	Total	O	0	0
			82	82		

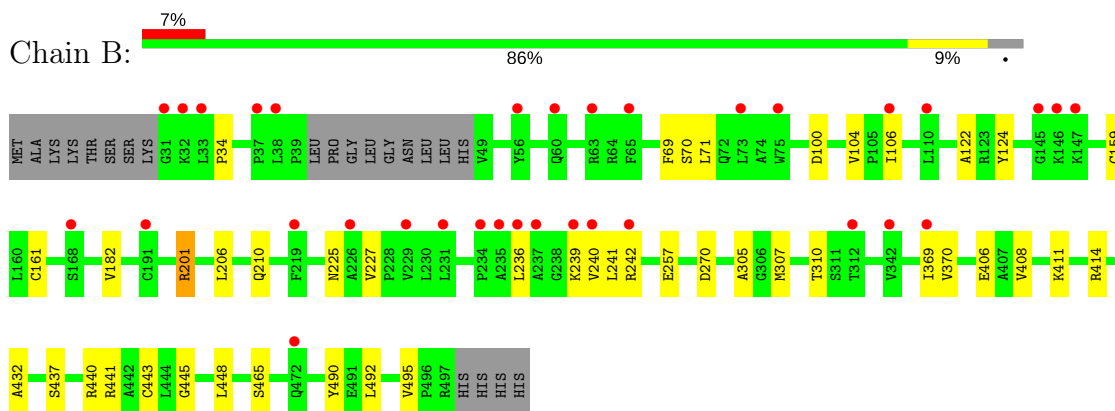
### 3 Residue-property plots [i](#)

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

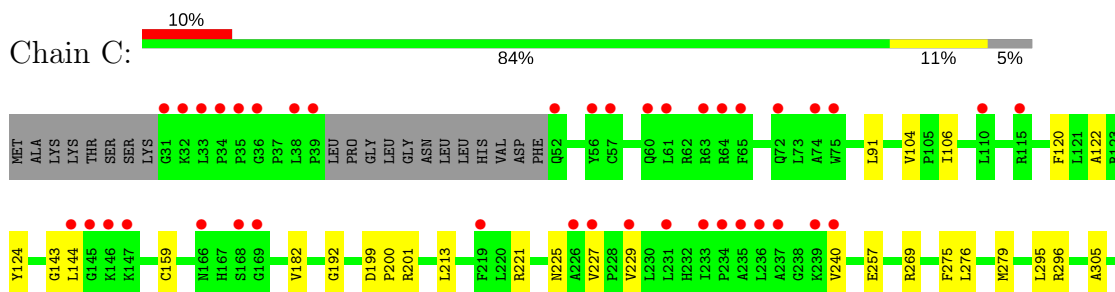
#### • Molecule 1: Cytochrome P450 2D6



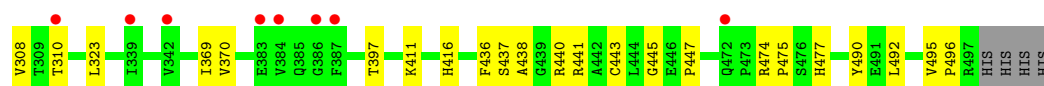
#### • Molecule 1: Cytochrome P450 2D6



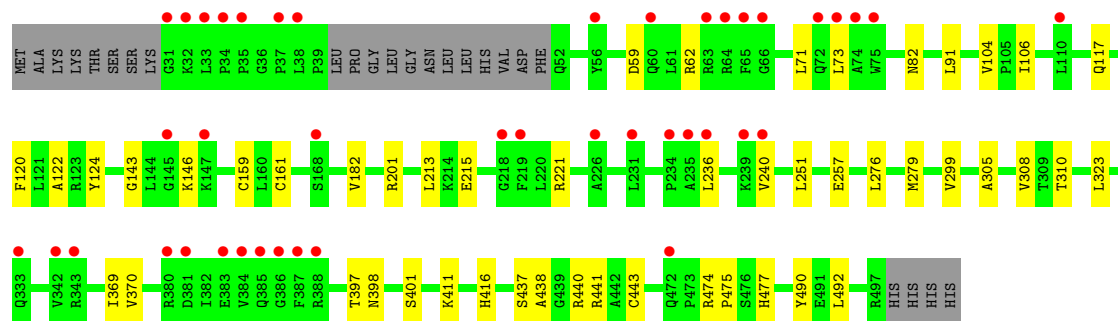
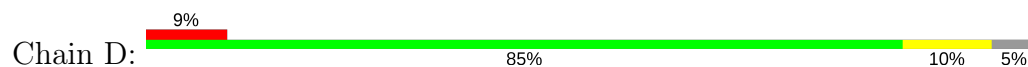
#### • Molecule 1: Cytochrome P450 2D6







● Molecule 1: Cytochrome P450 2D6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.54Å 192.48Å 244.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.93 – 2.40 38.93 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (38.93-2.40) 99.7 (38.93-2.40)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.217 , 0.254 0.219 , 0.256	Depositor DCC
$R_{free}$ test set	5369 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.704	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 56.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	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 21.08 % 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 7.5650e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, ZN, SI6, HEM, NA

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	0.21	0/3715	0.38	0/5050
1	B	0.21	0/3722	0.39	0/5060
1	C	0.21	0/3695	0.38	0/5023
1	D	0.21	0/3695	0.38	0/5023
All	All	0.21	0/14827	0.38	0/20156

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3618	0	3599	26	0
1	B	3625	0	3608	28	0
1	C	3599	0	3586	33	0
1	D	3599	0	3585	31	0
2	A	43	0	30	3	0
2	B	43	0	30	6	0
2	C	43	0	30	5	0
2	D	43	0	30	4	0
3	A	24	0	16	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	24	0	16	2	0
3	C	24	0	16	2	0
3	D	24	0	16	2	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	91	0	0	1	0
7	B	97	0	0	3	0
7	C	73	0	0	2	0
7	D	82	0	0	2	0
All	All	15092	0	14594	124	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 4.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:LEU:HD22	1:D:308:VAL:HG21	1.70	0.72
1:B:240:VAL:HG12	1:B:241:LEU:HG	1.71	0.71
1:A:122:ALA:O	1:A:441:ARG:NH2	2.20	0.67
1:A:62:ARG:HE	1:A:82:ASN:HB3	1.59	0.66
1:C:122:ALA:O	1:C:441:ARG:NH2	2.23	0.65
1:B:201:ARG:NH1	1:B:257:GLU:OE2	2.30	0.62
1:D:143:GLY:HA2	1:D:146:LYS:HE3	1.83	0.61
1:A:305:ALA:HB2	3:A:602:SI6:H8	1.83	0.61
1:C:369:ILE:HG13	1:C:370:VAL:HG23	1.84	0.59
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	1.85	0.58
1:B:305:ALA:HB2	3:B:602:SI6:H8	1.85	0.58
2:D:601:HEM:HMC2	2:D:601:HEM:HBC2	1.86	0.58
1:C:124:TYR:OH	1:C:440:ARG:NH2	2.35	0.58
1:B:182:VAL:HG11	1:B:310:THR:HB	1.84	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ILE:HD11	1:C:240:VAL:HG11	1.85	0.57
1:A:201:ARG:NH1	1:A:257:GLU:OE2	2.33	0.57
1:D:305:ALA:HB2	3:D:602:SI6:H8	1.87	0.56
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.88	0.56
1:D:122:ALA:O	1:D:441:ARG:NH2	2.23	0.56
1:D:104:VAL:HG12	1:D:106:ILE:HG22	1.87	0.56
1:B:210:GLN:HG2	1:B:307:MET:HE1	1.88	0.55
1:C:305:ALA:HB2	3:C:602:SI6:H8	1.87	0.55
1:B:104:VAL:HG12	1:B:106:ILE:HG22	1.88	0.55
1:B:159:CYS:SG	7:B:733:HOH:O	2.58	0.55
1:C:159:CYS:SG	7:C:730:HOH:O	2.58	0.55
2:D:601:HEM:HBB2	2:D:601:HEM:HMB1	1.89	0.55
1:A:91:LEU:HD11	1:A:397:THR:HG21	1.89	0.55
1:B:406:GLU:O	1:D:411:LYS:NZ	2.34	0.55
1:B:443:CYS:HB2	2:B:601:HEM:NA	2.20	0.55
1:C:201:ARG:NH1	1:C:257:GLU:OE1	2.33	0.55
1:B:161:CYS:SG	7:B:751:HOH:O	2.59	0.54
1:A:192:GLY:O	1:A:269:ARG:NH2	2.40	0.54
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.89	0.54
1:A:443:CYS:HB2	2:A:601:HEM:NA	2.21	0.54
1:C:279:MET:HE1	1:C:295:LEU:HD22	1.90	0.54
1:B:369:ILE:HG13	1:B:370:VAL:HG23	1.88	0.54
1:C:144:LEU:HD21	1:C:447:PRO:HB2	1.90	0.53
1:B:305:ALA:HB1	3:B:602:SI6:H16	1.89	0.53
2:B:601:HEM:HBB2	2:B:601:HEM:HMB1	1.90	0.52
1:B:34:PRO:HG2	1:B:70:SER:HB2	1.91	0.52
1:A:182:VAL:HG11	1:A:310:THR:HB	1.92	0.52
1:B:122:ALA:O	1:B:441:ARG:NH2	2.21	0.52
1:C:296:ARG:NH1	7:C:734:HOH:O	2.37	0.52
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.92	0.51
1:C:192:GLY:O	1:C:269:ARG:NH2	2.43	0.51
1:A:159:CYS:SG	7:A:749:HOH:O	2.59	0.51
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.92	0.51
1:D:443:CYS:HB2	2:D:601:HEM:NA	2.25	0.51
1:A:305:ALA:HB1	3:A:602:SI6:H16	1.92	0.51
1:B:239:LYS:HD2	1:B:242:ARG:HD2	1.92	0.51
1:A:369:ILE:HG13	1:A:370:VAL:HG23	1.92	0.50
1:D:411:LYS:HD2	1:D:416:HIS:CG	2.47	0.49
1:A:34:PRO:HG2	1:A:70:SER:HB2	1.93	0.49
1:D:124:TYR:OH	1:D:440:ARG:NH2	2.43	0.49
1:D:369:ILE:HG13	1:D:370:VAL:HG23	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:CYS:SG	7:D:762:HOH:O	2.60	0.48
1:D:201:ARG:NH1	1:D:257:GLU:OE1	2.33	0.48
1:C:437:SER:HB3	2:C:601:HEM:HBA1	1.94	0.48
1:D:161:CYS:SG	7:D:741:HOH:O	2.60	0.48
1:B:437:SER:HB3	2:B:601:HEM:HBA1	1.95	0.48
1:C:443:CYS:HB2	2:C:601:HEM:NA	2.27	0.48
1:C:276:LEU:HD23	1:C:279:MET:HE3	1.94	0.48
1:A:240:VAL:HG22	1:A:241:LEU:HG	1.96	0.47
1:A:490:TYR:HE1	1:A:492:LEU:HD23	1.79	0.47
1:C:213:LEU:HG	1:C:308:VAL:HG21	1.96	0.47
1:A:259:ARG:NH2	1:A:292:ASP:OD2	2.48	0.47
1:C:411:LYS:HD2	1:C:416:HIS:CG	2.50	0.47
1:D:323:LEU:HD13	1:D:477:HIS:CE1	2.50	0.47
1:C:305:ALA:HB1	3:C:602:SI6:H16	1.97	0.47
1:D:251:LEU:HD21	1:D:299:VAL:HG12	1.96	0.47
1:D:62:ARG:HD3	1:D:82:ASN:HB3	1.97	0.47
1:C:490:TYR:HE1	1:C:492:LEU:HD23	1.80	0.46
1:D:59:ASP:OD2	1:D:62:ARG:NH2	2.48	0.46
1:C:445:GLY:HA3	2:C:601:HEM:C3C	2.50	0.46
1:D:437:SER:HB3	2:D:601:HEM:HBA1	1.97	0.46
1:B:104:VAL:HG13	1:B:225:ASN:HD21	1.80	0.46
1:B:69:PHE:HE1	1:B:71:LEU:HD23	1.81	0.46
1:D:215:GLU:O	1:D:221:ARG:HD2	2.16	0.46
1:C:221:ARG:O	1:C:225:ASN:HB2	2.16	0.46
1:D:236:LEU:O	1:D:240:VAL:HG23	2.16	0.46
1:C:182:VAL:HG11	1:C:310:THR:HB	1.99	0.45
1:D:490:TYR:HE1	1:D:492:LEU:HD23	1.81	0.45
1:D:276:LEU:HD23	1:D:279:MET:HE3	1.99	0.45
1:C:276:LEU:HA	1:C:279:MET:HE3	1.99	0.44
1:A:411:LYS:HB3	1:A:414:ARG:HG3	1.99	0.44
1:D:117:GLN:HB3	1:D:122:ALA:HA	1.99	0.44
1:D:182:VAL:HG11	1:D:310:THR:HB	2.00	0.44
1:B:445:GLY:HA3	2:B:601:HEM:C3C	2.53	0.44
1:C:227:VAL:HG12	1:C:229:VAL:HG22	1.98	0.44
1:D:474:ARG:HA	1:D:475:PRO:HD3	1.81	0.44
1:C:437:SER:OG	1:C:438:ALA:N	2.47	0.44
1:A:71:LEU:HD12	1:A:78:VAL:HB	2.00	0.44
1:A:406:GLU:O	1:C:411:LYS:NZ	2.37	0.43
1:B:490:TYR:HE1	1:B:492:LEU:HD23	1.83	0.43
1:D:91:LEU:HD11	1:D:397:THR:HG21	2.00	0.43
1:B:206:LEU:HB3	1:B:307:MET:HE3	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:PHE:HB3	1:A:443:CYS:HB3	2.01	0.43
1:B:236:LEU:O	1:B:240:VAL:HG23	2.19	0.43
1:C:323:LEU:HD13	1:C:477:HIS:CE1	2.54	0.43
1:D:398:ASN:ND2	1:D:401:SER:HB3	2.33	0.43
1:C:199:ASP:HA	1:C:200:PRO:HD3	1.90	0.42
1:C:474:ARG:HA	1:C:475:PRO:HD3	1.80	0.42
1:C:104:VAL:HG12	1:C:106:ILE:HG22	1.99	0.42
1:C:275:PHE:HD2	1:C:279:MET:HE2	1.85	0.42
1:A:199:ASP:HB3	1:A:202:PHE:HB3	2.02	0.42
1:B:465:SER:HB3	1:B:495:VAL:HG23	2.01	0.42
1:D:305:ALA:HB1	3:D:602:SI6:H16	2.02	0.42
1:A:199:ASP:HA	1:A:200:PRO:HD3	1.91	0.41
1:C:436:PHE:HB3	1:C:443:CYS:HB3	2.01	0.41
1:B:100:ASP:HA	1:B:124:TYR:HB2	2.01	0.41
1:C:495:VAL:HA	1:C:496:PRO:HD3	1.95	0.41
1:B:440:ARG:NE	7:B:734:HOH:O	2.52	0.41
1:C:91:LEU:HD11	1:C:397:THR:HG21	2.01	0.41
1:D:71:LEU:HD22	1:D:73:LEU:HG	2.02	0.41
1:A:227:VAL:HA	1:A:228:PRO:HD3	1.87	0.41
1:A:406:GLU:HA	1:A:412:PRO:HG2	2.03	0.41
1:A:325:PRO:O	1:A:329:ARG:HG3	2.21	0.41
1:A:100:ASP:HA	1:A:124:TYR:HB2	2.03	0.40
1:A:233:ILE:HA	1:A:234:PRO:HD3	1.92	0.40
1:B:448:LEU:HD23	2:B:601:HEM:HBC2	2.03	0.40
1:D:276:LEU:HA	1:D:279:MET:HE3	2.04	0.40
1:B:411:LYS:HB3	1:B:414:ARG:HG3	2.03	0.40
1:B:408:VAL:HG11	1:B:432:ALA:HB3	2.04	0.40
1:D:437:SER:OG	1:D:438:ALA:N	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	453/479 (95%)	439 (97%)	14 (3%)	0	100	100
1	B	454/479 (95%)	440 (97%)	14 (3%)	0	100	100
1	C	451/479 (94%)	438 (97%)	12 (3%)	1 (0%)	49	65
1	D	451/479 (94%)	436 (97%)	15 (3%)	0	100	100
All	All	1809/1916 (94%)	1753 (97%)	55 (3%)	1 (0%)	53	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	143	GLY

### 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	390/409 (95%)	388 (100%)	2 (0%)	90	96
1	B	391/409 (96%)	388 (99%)	3 (1%)	83	92
1	C	388/409 (95%)	387 (100%)	1 (0%)	93	97
1	D	388/409 (95%)	387 (100%)	1 (0%)	93	97
All	All	1557/1636 (95%)	1550 (100%)	7 (0%)	92	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
1	A	344	ARG
1	B	201	ARG
1	B	227	VAL
1	B	270	ASP
1	C	120	PHE
1	D	120	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:



Mol	Chain	Res	Type
1	B	210	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](#)

Of 28 ligands modelled in this entry, 16 are monoatomic - leaving 12 for Mogul analysis.

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	601	1,3	27,50,50	1.72	4 (14%)	17,82,82	1.39	3 (17%)
3	SI6	A	602	2	23,27,27	1.31	4 (17%)	22,40,40	1.35	3 (13%)
5	GOL	A	606	-	5,5,5	0.37	0	5,5,5	0.23	0
2	HEM	B	601	1,3	27,50,50	1.69	4 (14%)	17,82,82	1.44	2 (11%)
3	SI6	B	602	2	23,27,27	1.35	4 (17%)	22,40,40	1.28	3 (13%)
5	GOL	B	605	-	5,5,5	0.35	0	5,5,5	0.27	0
2	HEM	C	601	1,3	27,50,50	1.68	4 (14%)	17,82,82	1.41	2 (11%)
3	SI6	C	602	2	23,27,27	1.24	3 (13%)	22,40,40	1.28	3 (13%)
5	GOL	C	606	-	5,5,5	0.35	0	5,5,5	0.31	0
2	HEM	D	601	1,3	27,50,50	1.69	4 (14%)	17,82,82	1.45	3 (17%)
3	SI6	D	602	2	23,27,27	1.21	3 (13%)	22,40,40	1.35	3 (13%)
5	GOL	D	606	-	5,5,5	0.37	0	5,5,5	0.25	0

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	601	1,3	-	0/6/54/54	0/0/8/8
3	SI6	A	602	2	-	0/5/36/36	0/4/4/4
5	GOL	A	606	-	-	0/4/4/4	0/0/0/0
2	HEM	B	601	1,3	-	0/6/54/54	0/0/8/8
3	SI6	B	602	2	-	0/5/36/36	0/4/4/4
5	GOL	B	605	-	-	0/4/4/4	0/0/0/0
2	HEM	C	601	1,3	-	0/6/54/54	0/0/8/8
3	SI6	C	602	2	-	0/5/36/36	0/4/4/4
5	GOL	C	606	-	-	0/4/4/4	0/0/0/0
2	HEM	D	601	1,3	-	0/6/54/54	0/0/8/8
3	SI6	D	602	2	-	0/5/36/36	0/4/4/4
5	GOL	D	606	-	-	0/4/4/4	0/0/0/0

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3C-C2C	-3.72	1.35	1.40
2	B	601	HEM	C3C-C2C	-3.68	1.35	1.40
2	C	601	HEM	C3C-C2C	-3.65	1.35	1.40
2	D	601	HEM	C3C-C2C	-3.56	1.35	1.40
2	C	601	HEM	C3B-C2B	-3.54	1.35	1.40
2	A	601	HEM	C3B-C2B	-3.51	1.35	1.40
2	B	601	HEM	C3B-C2B	-3.47	1.35	1.40
2	D	601	HEM	C3B-C2B	-3.47	1.35	1.40
3	B	602	SI6	C12-C11	-2.66	1.50	1.52
3	D	602	SI6	C3-C4	2.01	1.41	1.38
3	B	602	SI6	C15-N3	2.02	1.39	1.33
3	D	602	SI6	C15-N3	2.02	1.39	1.33
3	C	602	SI6	C15-N3	2.02	1.39	1.33
3	A	602	SI6	C15-N3	2.04	1.39	1.33
3	C	602	SI6	C3-C4	2.06	1.41	1.38
3	A	602	SI6	C12-C11	2.06	1.54	1.52
3	B	602	SI6	C3-C4	2.23	1.42	1.38
3	A	602	SI6	C3-C4	2.29	1.42	1.38
3	D	602	SI6	C16-C14	2.31	1.43	1.37
3	C	602	SI6	C16-C14	2.36	1.43	1.37
3	B	602	SI6	C16-C14	2.36	1.43	1.37
3	A	602	SI6	C16-C14	2.42	1.43	1.37
2	C	601	HEM	C3B-CAB	3.85	1.55	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HEM	C3B-CAB	3.87	1.55	1.47
2	D	601	HEM	C3B-CAB	3.88	1.55	1.47
2	A	601	HEM	C3B-CAB	3.96	1.55	1.47
2	C	601	HEM	C3C-CAC	4.04	1.55	1.47
2	B	601	HEM	C3C-CAC	4.09	1.55	1.47
2	D	601	HEM	C3C-CAC	4.15	1.56	1.47
2	A	601	HEM	C3C-CAC	4.15	1.56	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	SI6	O1-C9-C14	-2.42	105.23	108.50
3	A	602	SI6	O1-C9-C14	-2.24	105.47	108.50
3	B	602	SI6	O1-C9-C14	-2.19	105.53	108.50
3	C	602	SI6	O1-C9-C14	-2.16	105.57	108.50
2	D	601	HEM	CAA-CBA-CGA	-2.10	109.08	112.66
2	A	601	HEM	CAA-CBA-CGA	-2.03	109.19	112.66
2	A	601	HEM	CMB-C2B-C3B	2.02	128.56	124.88
2	C	601	HEM	CMC-C2C-C3C	2.08	128.66	124.88
2	B	601	HEM	CMC-C2C-C3C	2.11	128.73	124.88
2	A	601	HEM	CMC-C2C-C3C	2.15	128.80	124.88
2	B	601	HEM	CMB-C2B-C3B	2.16	128.81	124.88
2	D	601	HEM	CMB-C2B-C3B	2.16	128.82	124.88
3	B	602	SI6	C11-C7-N1	2.17	113.26	109.70
2	C	601	HEM	CMB-C2B-C3B	2.23	128.94	124.88
2	D	601	HEM	CMC-C2C-C3C	2.24	128.95	124.88
3	C	602	SI6	C11-C7-N1	2.39	113.64	109.70
3	D	602	SI6	C11-C7-N1	2.43	113.69	109.70
3	A	602	SI6	C11-C7-N1	2.44	113.72	109.70
3	C	602	SI6	F2-C4-C3	3.06	122.36	118.93
3	D	602	SI6	F2-C4-C3	3.12	122.42	118.93
3	B	602	SI6	F2-C4-C3	3.20	122.51	118.93
3	A	602	SI6	F2-C4-C3	3.21	122.53	118.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	SI6	2	0
2	B	601	HEM	6	0
3	B	602	SI6	2	0
2	C	601	HEM	5	0
3	C	602	SI6	2	0
2	D	601	HEM	4	0
3	D	602	SI6	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	457/479 (95%)	0.30	40 (8%) 10 9	23, 43, 90, 109	0
1	B	458/479 (95%)	0.28	33 (7%) 15 14	23, 42, 90, 118	0
1	C	455/479 (94%)	0.52	48 (10%) 6 5	26, 47, 96, 114	0
1	D	455/479 (94%)	0.38	42 (9%) 9 8	24, 44, 90, 110	0
All	All	1825/1916 (95%)	0.37	163 (8%) 9 8	23, 44, 92, 118	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	TYR	9.2
1	D	73	LEU	8.8
1	A	75	TRP	8.7
1	D	75	TRP	8.0
1	C	219	PHE	7.6
1	D	74	ALA	7.5
1	C	33	LEU	7.3
1	C	145	GLY	7.0
1	D	342	VAL	6.8
1	D	33	LEU	6.8
1	D	31	GLY	6.5
1	C	75	TRP	6.3
1	C	31	GLY	5.8
1	B	75	TRP	5.7
1	D	145	GLY	5.5
1	D	32	LYS	5.4
1	C	64	ARG	5.3
1	C	227	VAL	5.2
1	A	219	PHE	5.1
1	C	236	LEU	5.1
1	C	32	LYS	5.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	145	GLY	4.9
1	B	33	LEU	4.7
1	D	219	PHE	4.7
1	C	110	LEU	4.7
1	A	32	LYS	4.7
1	A	147	LYS	4.6
1	B	234	PRO	4.5
1	C	60	GLN	4.5
1	D	60	GLN	4.5
1	C	229	VAL	4.5
1	C	234	PRO	4.4
1	A	64	ARG	4.4
1	A	31	GLY	4.4
1	C	38	LEU	4.3
1	D	110	LEU	4.3
1	B	219	PHE	4.2
1	D	387	PHE	4.1
1	C	386	GLY	4.1
1	B	342	VAL	4.1
1	A	145	GLY	4.0
1	B	235	ALA	4.0
1	B	38	LEU	4.0
1	B	60	GLN	4.0
1	C	147	LYS	3.9
1	C	240	VAL	3.9
1	C	65	PHE	3.9
1	B	31	GLY	3.9
1	B	110	LEU	3.8
1	A	33	LEU	3.8
1	C	342	VAL	3.8
1	C	237	ALA	3.8
1	D	226	ALA	3.8
1	D	56	TYR	3.7
1	A	60	GLN	3.7
1	B	56	TYR	3.7
1	C	472	GLN	3.6
1	A	38	LEU	3.6
1	C	235	ALA	3.5
1	D	383	GLU	3.5
1	D	386	GLY	3.5
1	A	168	SER	3.5
1	A	342	VAL	3.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	169	GLY	3.4
1	A	234	PRO	3.3
1	D	235	ALA	3.3
1	C	168	SER	3.3
1	C	63	ARG	3.2
1	B	231	LEU	3.2
1	C	146	LYS	3.1
1	B	65	PHE	3.1
1	D	35	PRO	3.1
1	D	38	LEU	3.1
1	C	166	ASN	3.1
1	A	74	ALA	3.1
1	B	237	ALA	3.1
1	D	380	ARG	3.1
1	D	34	PRO	3.0
1	B	191	CYS	3.0
1	A	63	ARG	3.0
1	B	147	LYS	2.9
1	A	66	GLY	2.9
1	D	147	LYS	2.9
1	B	32	LYS	2.9
1	B	73	LEU	2.9
1	D	63	ARG	2.9
1	C	233	ILE	2.9
1	B	146	LYS	2.8
1	B	242	ARG	2.8
1	A	52	GLN	2.8
1	D	240	VAL	2.8
1	A	37	PRO	2.8
1	D	388	ARG	2.8
1	B	472	GLN	2.7
1	C	384	VAL	2.7
1	D	239	LYS	2.7
1	C	34	PRO	2.7
1	A	110	LEU	2.7
1	A	238	GLY	2.7
1	C	115	ARG	2.6
1	A	339	ILE	2.6
1	B	37	PRO	2.6
1	D	168	SER	2.6
1	A	146	LYS	2.6
1	C	387	PHE	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	2.6
1	D	218	GLY	2.6
1	A	39	PRO	2.6
1	A	169	GLY	2.6
1	C	383	GLU	2.6
1	D	384	VAL	2.5
1	D	385	GLN	2.5
1	D	64	ARG	2.5
1	C	39	PRO	2.5
1	C	310	THR	2.5
1	C	231	LEU	2.4
1	D	37	PRO	2.4
1	B	369	ILE	2.4
1	B	226	ALA	2.4
1	A	96	GLU	2.4
1	B	240	VAL	2.4
1	A	383	GLU	2.4
1	A	56	TYR	2.4
1	C	36	GLY	2.3
1	D	66	GLY	2.3
1	D	333	GLN	2.3
1	A	36	GLY	2.3
1	A	338	VAL	2.3
1	B	63	ARG	2.3
1	A	236	LEU	2.3
1	A	76	THR	2.3
1	A	58	PHE	2.3
1	A	72	GLN	2.3
1	A	386	GLY	2.3
1	D	234	PRO	2.2
1	B	236	LEU	2.2
1	A	237	ALA	2.2
1	A	387	PHE	2.2
1	A	191	CYS	2.2
1	C	57	CYS	2.2
1	B	312	THR	2.2
1	D	65	PHE	2.2
1	C	35	PRO	2.2
1	D	236	LEU	2.2
1	D	472	GLN	2.2
1	D	343	ARG	2.2
1	C	61	LEU	2.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	381	ASP	2.1
1	B	239	LYS	2.1
1	C	72	GLN	2.1
1	D	72	GLN	2.1
1	B	106	ILE	2.1
1	C	339	ILE	2.1
1	C	226	ALA	2.1
1	B	168	SER	2.1
1	C	144	LEU	2.1
1	A	226	ALA	2.0
1	A	54	THR	2.0
1	A	65	PHE	2.0
1	C	74	ALA	2.0
1	C	239	LYS	2.0
1	B	229	VAL	2.0
1	C	52	GLN	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	C	606	6/6	0.64	0.28	44,53,58,66	0
5	GOL	A	606	6/6	0.73	0.27	44,47,49,49	0
4	ZN	A	607	1/1	0.74	0.09	67,67,67,67	1
4	ZN	C	604	1/1	0.75	0.06	80,80,80,80	0
4	ZN	A	604	1/1	0.78	0.09	72,72,72,72	0
4	ZN	D	604	1/1	0.79	0.07	78,78,78,78	0
5	GOL	D	606	6/6	0.79	0.21	46,51,55,61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	605	6/6	0.83	0.24	32,48,53,56	0
4	ZN	C	605	1/1	0.85	0.06	77,77,77,77	0
4	ZN	D	605	1/1	0.90	0.10	81,81,81,81	0
6	NA	B	606	1/1	0.94	0.17	42,42,42,42	0
3	SI6	A	602	24/24	0.95	0.17	22,36,42,43	0
6	NA	A	608	1/1	0.96	0.09	50,50,50,50	0
3	SI6	B	602	24/24	0.96	0.17	18,36,41,51	0
6	NA	D	607	1/1	0.96	0.18	42,42,42,42	0
3	SI6	D	602	24/24	0.96	0.18	26,35,41,47	0
3	SI6	C	602	24/24	0.97	0.17	26,36,49,56	0
4	ZN	B	604	1/1	0.98	0.04	67,67,67,67	0
2	HEM	D	601	43/43	0.98	0.18	21,28,34,35	0
6	NA	C	607	1/1	0.98	0.10	50,50,50,50	0
2	HEM	B	601	43/43	0.98	0.20	22,28,34,37	0
4	ZN	C	603	1/1	0.99	0.11	30,30,30,30	0
4	ZN	A	603	1/1	0.99	0.11	31,31,31,31	0
2	HEM	A	601	43/43	0.99	0.19	17,25,31,32	0
4	ZN	B	603	1/1	0.99	0.13	32,32,32,32	0
4	ZN	A	605	1/1	0.99	0.10	46,46,46,46	0
4	ZN	D	603	1/1	0.99	0.10	31,31,31,31	0
2	HEM	C	601	43/43	0.99	0.18	21,29,34,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.