



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 12:13 pm GMT

PDB ID : 4XRY  
Title : Human Cytochrome P450 2D6 BACE1 Inhibitor 5 Complex  
Authors : Johnson, E.F.; Fan, Y.  
Deposited on : 2015-01-21  
Resolution : 2.50 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 : trunk31020  
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) : trunk31020

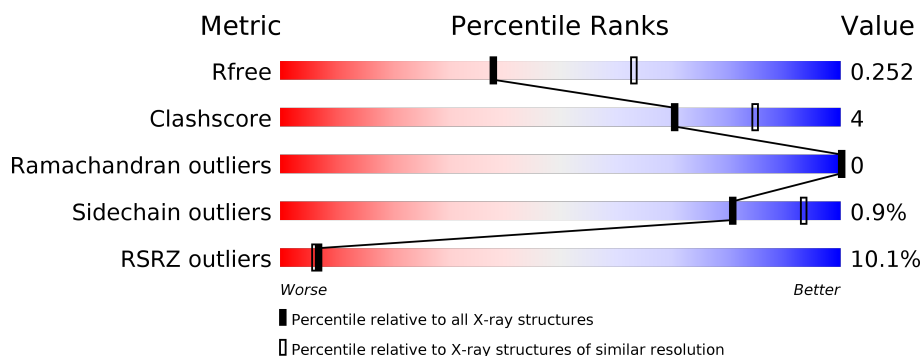
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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. 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>10%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>
1	B	479	<div> <div>6%</div> <div>85%</div> <div>9%</div> <div>5%</div> </div>
1	C	479	<div> <div>11%</div> <div>82%</div> <div>11%</div> <div>7%</div> </div>
1	D	479	<div> <div>11%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14847 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	464	Total	C	N	O	S	0	0	0
			3662	2349	649	650	14			
1	B	455	Total	C	N	O	S	0	0	0
			3602	2310	639	639	14			
1	C	446	Total	C	N	O	S	0	0	0
			3535	2267	625	629	14			
1	D	452	Total	C	N	O	S	0	0	0
			3577	2295	633	635	14			

There are 60 discrepancies between the modelled and reference sequences:

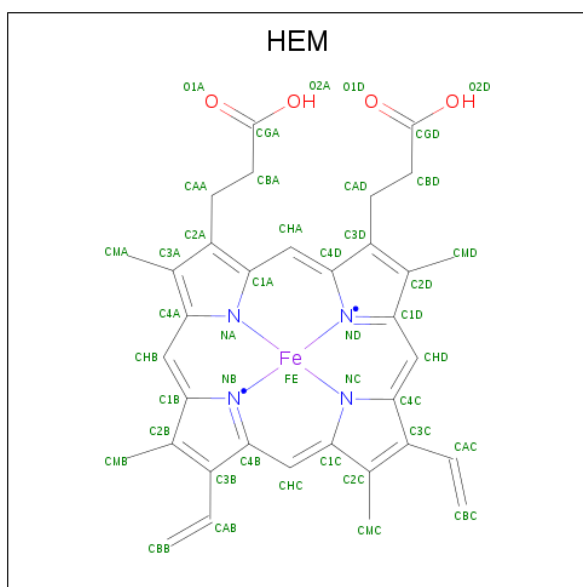
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP P10635
A	24	ALA	-	expression tag	UNP P10635
A	25	LYS	-	expression tag	UNP P10635
A	26	LYS	-	expression tag	UNP P10635
A	27	THR	-	expression tag	UNP P10635
A	28	SER	-	expression tag	UNP P10635
A	29	SER	-	expression tag	UNP P10635
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...*

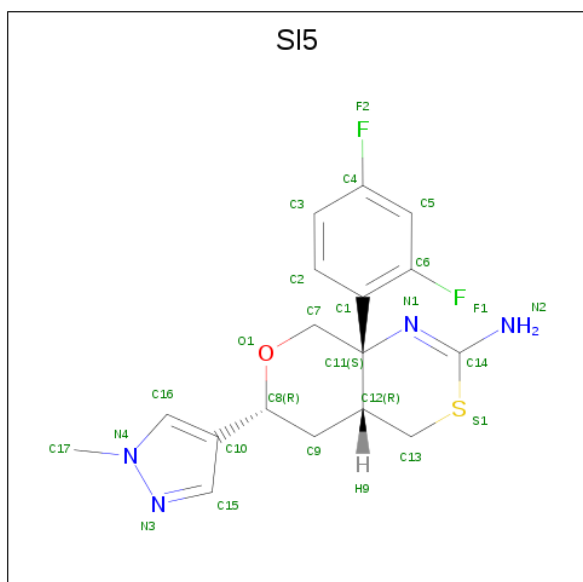
Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP P10635
B	30	LYS	-	expression tag	UNP P10635
B	31	GLY	-	expression tag	UNP P10635
B	32	LYS	-	expression tag	UNP P10635
B	33	LEU	-	expression tag	UNP P10635
B	498	HIS	-	expression tag	UNP P10635
B	499	HIS	-	expression tag	UNP 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-(1-methyl-1H-pyrazol-4-yl)-4,4a,5,6,8,8a-hexahydropyrano[3,4-d][1,3]thiazin-2-amine (three-letter code: SI5) (formula: C<sub>17</sub>H<sub>18</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	
			25	17	2	4	1	1	
3	B	1	Total	C	F	N	O	S	
			25	17	2	4	1	1	
3	C	1	Total	C	F	N	O	S	
			25	17	2	4	1	1	
3	D	1	Total	C	F	N	O	S	
			25	17	2	4	1	1	

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Zn		
			3	3	0	0
4	A	4	Total	Zn		
			4	4	0	0
4	D	5	Total	Zn		
			5	5	0	0
4	C	5	Total	Zn		
			5	5	0	0

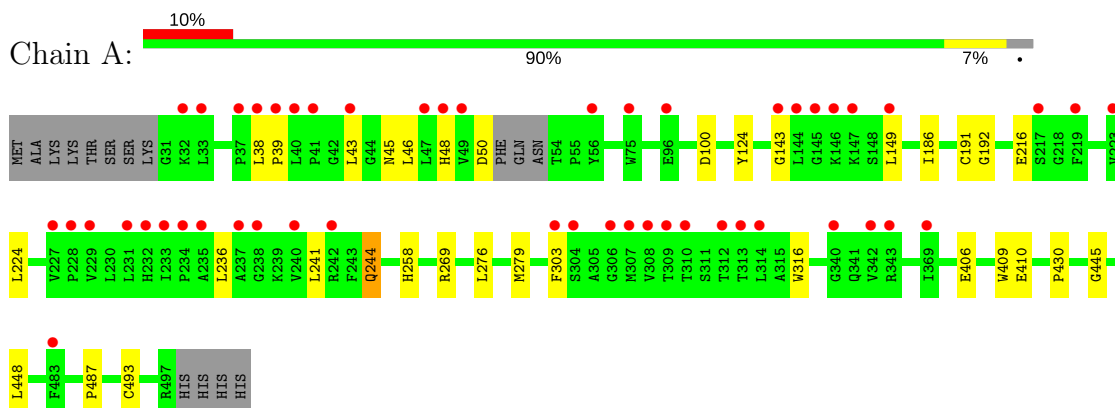
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O		
			54	54	0	0
5	B	43	Total	O		
			43	43	0	0
5	C	47	Total	O		
			47	47	0	0
5	D	38	Total	O		
			38	38	0	0

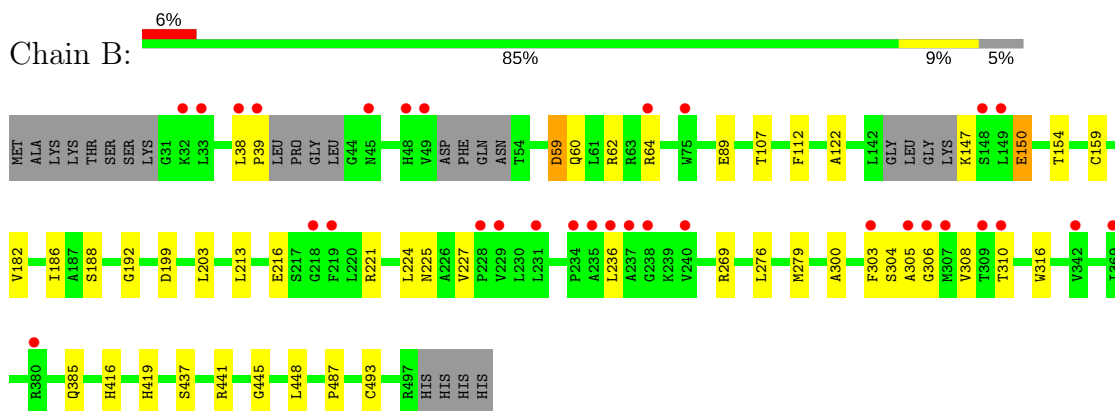
### 3 Residue-property plots

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

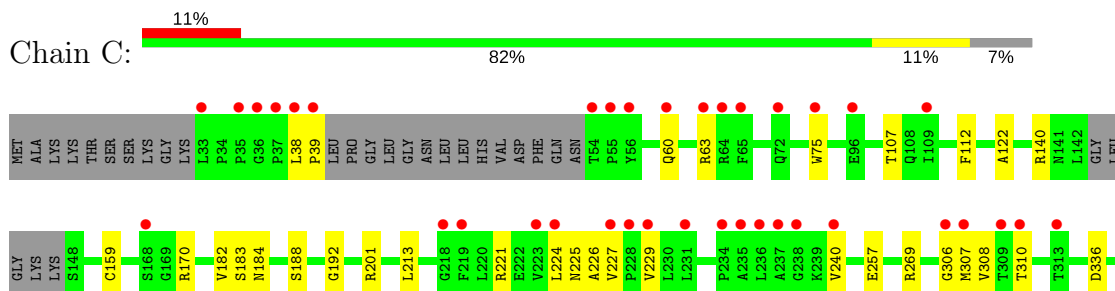
#### • Molecule 1: Cytochrome P450 2D6

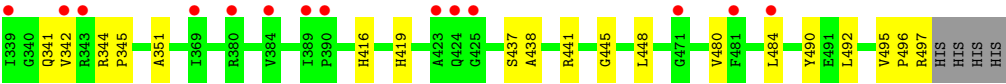


#### • Molecule 1: Cytochrome P450 2D6

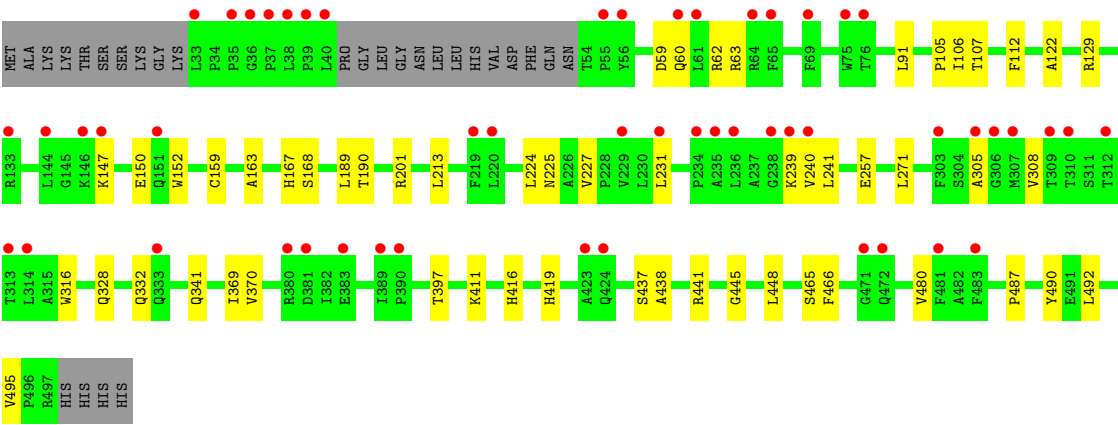
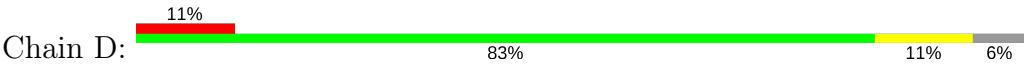


#### • Molecule 1: Cytochrome P450 2D6





● 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, $\alpha$ , $\beta$ , $\gamma$	57.06Å 192.34Å 247.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.16 – 2.50 39.16 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.16-2.50) 99.5 (39.16-2.50)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.208 , 0.251 0.214 , 0.252	Depositor DCC
$R_{free}$ test set	4767 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.652	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 59.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14847	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	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 21.69 % 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 6.6474e-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: HEM, ZN, SI5

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	0.23	0/3760	0.40	0/5113
1	B	0.23	0/3697	0.39	0/5025
1	C	0.22	0/3630	0.39	0/4938
1	D	0.22	0/3673	0.38	0/4995
All	All	0.22	0/14760	0.39	0/20071

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	3662	0	3654	21	0
1	B	3602	0	3586	27	0
1	C	3535	0	3510	28	0
1	D	3577	0	3565	35	0
2	A	43	0	30	4	0
2	B	43	0	30	6	0
2	C	43	0	30	6	0
2	D	43	0	30	4	0
3	A	25	0	18	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	18	1	0
3	C	25	0	18	0	0
3	D	25	0	18	2	0
4	A	4	0	0	0	0
4	B	3	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	54	0	0	1	0
5	B	43	0	0	2	0
5	C	47	0	0	3	0
5	D	38	0	0	3	0
All	All	14847	0	14507	115	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 (115) 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:A:186:ILE:HG21	1:A:303:PHE:HA	1.67	0.75
1:D:122:ALA:O	1:D:441:ARG:NH2	2.18	0.74
1:B:159:CYS:SG	5:B:713:HOH:O	2.44	0.74
1:C:122:ALA:O	1:C:441:ARG:NH2	2.18	0.74
1:B:493:CYS:SG	5:B:710:HOH:O	2.49	0.71
1:C:159:CYS:SG	5:C:715:HOH:O	2.51	0.69
1:B:186:ILE:HG21	1:B:303:PHE:HA	1.75	0.68
1:C:221:ARG:O	1:C:225:ASN:ND2	2.25	0.68
1:B:60:GLN:OE1	1:B:64:ARG:NH2	2.29	0.66
1:D:240:VAL:HG22	1:D:241:LEU:HG	1.79	0.65
1:D:416:HIS:ND1	5:D:715:HOH:O	2.29	0.65
1:C:60:GLN:OE1	1:C:63:ARG:NH1	2.31	0.63
1:B:38:LEU:HD12	1:B:39:PRO:HD2	1.83	0.61
1:C:140:ARG:NH1	5:C:744:HOH:O	2.29	0.60
1:C:224:LEU:HD12	1:C:240:VAL:HG11	1.82	0.60
1:D:147:LYS:HG2	1:D:150:GLU:HB2	1.84	0.59
2:A:601:HEM:HMB2	2:A:601:HEM:HBB2	1.85	0.58
1:A:192:GLY:O	1:A:269:ARG:NH2	2.33	0.57
1:D:159:CYS:SG	5:D:712:HOH:O	2.58	0.56
1:D:437:SER:HB3	2:D:601:HEM:HBA1	1.86	0.56
1:D:437:SER:OG	1:D:438:ALA:N	2.35	0.56
1:A:493:CYS:SG	5:A:730:HOH:O	2.57	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ALA:O	1:B:441:ARG:NH2	2.18	0.54
1:C:437:SER:HB3	2:C:601:HEM:HBA1	1.89	0.54
2:A:601:HEM:HMC2	2:A:601:HEM:HBC2	1.90	0.53
1:C:213:LEU:HD11	1:C:484:LEU:HD12	1.91	0.53
1:B:216:GLU:HA	1:B:221:ARG:HD3	1.90	0.53
1:C:227:VAL:HG12	1:C:229:VAL:HG22	1.91	0.53
1:C:437:SER:OG	1:C:438:ALA:N	2.34	0.52
1:D:213:LEU:HD12	3:D:602:SI5:H4	1.91	0.52
1:A:241:LEU:HB3	1:A:244:GLN:HB2	1.92	0.52
2:C:601:HEM:HMB2	2:C:601:HEM:HBB2	1.91	0.52
1:B:300:ALA:O	1:B:304:SER:OG	2.27	0.52
1:A:43:LEU:HD23	1:A:46:LEU:HD22	1.91	0.51
1:D:106:ILE:HD12	1:D:241:LEU:HD11	1.92	0.51
1:C:184:ASN:O	1:C:188:SER:OG	2.24	0.51
1:B:192:GLY:O	1:B:269:ARG:NH2	2.41	0.51
1:C:183:SER:OG	1:C:307:MET:HG3	2.10	0.51
2:D:601:HEM:HBB2	2:D:601:HEM:HMB2	1.91	0.51
1:A:276:LEU:HD23	1:A:279:MET:HE3	1.93	0.50
1:C:445:GLY:HA3	2:C:601:HEM:C3C	2.47	0.50
1:C:336:ASP:OD2	1:C:497:ARG:NH2	2.43	0.50
1:A:191:CYS:HA	1:A:258:HIS:CE1	2.47	0.49
2:B:601:HEM:HBC2	2:B:601:HEM:HMC2	1.94	0.49
1:B:437:SER:HB3	2:B:601:HEM:HBA1	1.94	0.49
1:D:59:ASP:O	1:D:63:ARG:HG2	2.13	0.49
1:B:448:LEU:HD23	2:B:601:HEM:HBC2	1.94	0.48
1:D:129:ARG:NH1	5:D:732:HOH:O	2.45	0.48
1:D:201:ARG:NH1	1:D:257:GLU:OE1	2.32	0.48
1:D:448:LEU:HD23	2:D:601:HEM:HBC2	1.96	0.48
2:B:601:HEM:HMB2	2:B:601:HEM:HBB2	1.95	0.47
1:D:316:TRP:CD2	1:D:487:PRO:HG3	2.50	0.47
1:B:147:LYS:HE3	1:B:150:GLU:HB2	1.96	0.47
1:A:224:LEU:HD21	1:A:236:LEU:HD13	1.96	0.47
1:D:490:TYR:HE1	1:D:492:LEU:HD23	1.80	0.47
1:B:182:VAL:HG11	1:B:310:THR:HB	1.96	0.46
1:A:50:ASP:OD2	1:D:60:GLN:NE2	2.49	0.46
1:B:107:THR:HB	1:B:112:PHE:CG	2.51	0.46
1:A:241:LEU:HD22	1:A:244:GLN:HG3	1.97	0.46
1:A:38:LEU:HA	1:A:39:PRO:HD3	1.77	0.46
1:C:192:GLY:O	1:C:269:ARG:NH2	2.49	0.45
1:C:201:ARG:NH1	1:C:257:GLU:OE1	2.39	0.45
1:D:213:LEU:HD13	1:D:308:VAL:HG21	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:O	1:B:225:ASN:HB2	2.16	0.45
1:B:89:GLU:OE2	1:B:385:GLN:NE2	2.39	0.45
1:C:182:VAL:HG11	1:C:310:THR:HB	1.99	0.45
1:A:216:GLU:OE2	3:A:602:SI5:N2	2.42	0.44
1:D:369:ILE:HG13	1:D:370:VAL:HG23	1.98	0.44
1:C:75:TRP:CZ2	1:C:226:ALA:HB2	2.52	0.44
1:C:306:GLY:HA2	2:C:601:HEM:C2C	2.53	0.44
1:C:490:TYR:HE1	1:C:492:LEU:HD23	1.83	0.44
1:D:328:GLN:OE1	1:D:466:PHE:N	2.43	0.44
2:C:601:HEM:HMC2	2:C:601:HEM:HBC2	2.00	0.44
1:D:316:TRP:CG	1:D:487:PRO:HG3	2.52	0.44
1:D:163:ALA:O	1:D:167:HIS:ND1	2.40	0.44
1:A:100:ASP:HA	1:A:124:TYR:HB2	1.99	0.44
1:B:305:ALA:HB2	3:B:602:SI5:H8	2.00	0.44
1:D:224:LEU:HB3	1:D:231:LEU:HD21	2.00	0.43
1:C:107:THR:HB	1:C:112:PHE:CG	2.53	0.43
1:D:416:HIS:HB3	1:D:419:HIS:CE1	2.53	0.43
1:A:410:GLU:O	1:D:411:LYS:NZ	2.46	0.43
1:A:143:GLY:HA2	1:A:149:LEU:HD13	1.99	0.43
1:B:213:LEU:HD22	1:B:308:VAL:HG21	1.99	0.43
1:A:45:ASN:HA	1:A:48:HIS:HD2	1.84	0.43
1:C:495:VAL:HA	1:C:496:PRO:HD3	1.88	0.43
1:B:224:LEU:HD11	1:B:236:LEU:HD23	1.99	0.43
1:D:190:THR:HA	1:D:271:LEU:HB3	2.01	0.43
1:D:465:SER:HB3	1:D:495:VAL:HG23	2.01	0.43
1:C:213:LEU:HD13	1:C:308:VAL:HG21	2.00	0.42
1:B:445:GLY:HA3	2:B:601:HEM:C3C	2.54	0.42
1:C:416:HIS:HB3	1:C:419:HIS:CE1	2.53	0.42
1:A:406:GLU:O	1:D:411:LYS:HE3	2.19	0.42
1:B:416:HIS:HB3	1:B:419:HIS:CE1	2.54	0.42
1:B:199:ASP:O	1:B:203:LEU:HG	2.20	0.42
1:C:38:LEU:HD12	1:C:39:PRO:HD2	2.01	0.42
1:B:316:TRP:CD2	1:B:487:PRO:HG3	2.54	0.42
1:B:59:ASP:HA	1:B:62:ARG:HG2	2.02	0.42
1:C:344:ARG:HA	1:C:345:PRO:HD3	1.92	0.41
1:D:332:GLN:HE22	1:D:465:SER:HA	1.86	0.41
1:A:409:TRP:CZ3	1:A:430:PRO:HG2	2.55	0.41
1:A:448:LEU:HD23	2:A:601:HEM:HBC2	2.02	0.41
1:D:91:LEU:HD11	1:D:397:THR:HG21	2.02	0.41
1:A:316:TRP:CG	1:A:487:PRO:HG3	2.56	0.41
1:B:150:GLU:O	1:B:154:THR:HG23	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLY:HA2	2:B:601:HEM:C2C	2.55	0.41
1:C:351:ALA:N	5:C:724:HOH:O	2.45	0.41
1:D:445:GLY:HA3	2:D:601:HEM:C3C	2.56	0.41
1:A:445:GLY:HA3	2:A:601:HEM:C3C	2.55	0.40
1:D:107:THR:HB	1:D:112:PHE:CG	2.55	0.40
1:D:239:LYS:HB3	1:D:239:LYS:HE2	1.84	0.40
1:B:276:LEU:HA	1:B:279:MET:HE3	2.04	0.40
1:C:448:LEU:HD23	2:C:601:HEM:HBC2	2.03	0.40
1:D:152:TRP:CZ3	1:D:189:LEU:HD23	2.56	0.40
1:D:305:ALA:HB2	3:D:602:SI5:H8	2.03	0.40
1:D:105:PRO:HD2	1:D:225:ASN:OD1	2.22	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	460/479 (96%)	446 (97%)	14 (3%)	0	100	100
1	B	447/479 (93%)	437 (98%)	10 (2%)	0	100	100
1	C	440/479 (92%)	427 (97%)	13 (3%)	0	100	100
1	D	448/479 (94%)	435 (97%)	13 (3%)	0	100	100
All	All	1795/1916 (94%)	1745 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	395/409 (97%)	394 (100%)	1 (0%)	93	98
1	B	389/409 (95%)	385 (99%)	4 (1%)	78	92
1	C	382/409 (93%)	378 (99%)	4 (1%)	78	92
1	D	386/409 (94%)	381 (99%)	5 (1%)	71	89
All	All	1552/1636 (95%)	1538 (99%)	14 (1%)	81	93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	GLN
1	B	59	ASP
1	B	150	GLU
1	B	188	SER
1	B	227	VAL
1	C	170	ARG
1	C	341	GLN
1	C	342	VAL
1	C	480	VAL
1	D	62	ARG
1	D	168	SER
1	D	227	VAL
1	D	341	GLN
1	D	480	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	C	332	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](#)

Of 25 ligands modelled in this entry, 17 are monoatomic - leaving 8 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	27,50,50	1.68	4 (14%)	17,82,82	1.52	3 (17%)
3	SI5	A	602	-	23,28,28	0.91	1 (4%)	26,42,42	1.05	2 (7%)
2	HEM	B	601	1,5	27,50,50	1.70	4 (14%)	17,82,82	1.46	4 (23%)
3	SI5	B	602	-	23,28,28	0.90	2 (8%)	26,42,42	1.12	2 (7%)
2	HEM	C	601	1	27,50,50	1.71	4 (14%)	17,82,82	1.52	4 (23%)
3	SI5	C	602	-	23,28,28	0.91	1 (4%)	26,42,42	1.10	2 (7%)
2	HEM	D	601	1,5	27,50,50	1.70	4 (14%)	17,82,82	1.50	3 (17%)
3	SI5	D	602	-	23,28,28	0.89	1 (4%)	26,42,42	1.19	2 (7%)

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	-	0/6/54/54	0/0/8/8
3	SI5	A	602	-	-	0/5/36/36	0/4/4/4
2	HEM	B	601	1,5	-	0/6/54/54	0/0/8/8
3	SI5	B	602	-	-	0/5/36/36	0/4/4/4
2	HEM	C	601	1	-	0/6/54/54	0/0/8/8
3	SI5	C	602	-	-	0/5/36/36	0/4/4/4
2	HEM	D	601	1,5	-	0/6/54/54	0/0/8/8
3	SI5	D	602	-	-	0/5/36/36	0/4/4/4

All (21) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	HEM	C3B-C2B	-3.72	1.35	1.40
2	C	601	HEM	C3C-C2C	-3.69	1.35	1.40
2	A	601	HEM	C3B-C2B	-3.68	1.35	1.40
2	D	601	HEM	C3B-C2B	-3.66	1.35	1.40
2	B	601	HEM	C3C-C2C	-3.60	1.35	1.40
2	D	601	HEM	C3C-C2C	-3.56	1.35	1.40
2	A	601	HEM	C3C-C2C	-3.53	1.35	1.40
2	B	601	HEM	C3B-C2B	-3.52	1.35	1.40
3	B	602	SI5	O1-C8	-2.07	1.40	1.43
3	D	602	SI5	C15-C10	2.10	1.43	1.37
3	B	602	SI5	C15-C10	2.11	1.43	1.37
3	C	602	SI5	C15-C10	2.18	1.43	1.37
3	A	602	SI5	C15-C10	2.24	1.43	1.37
2	A	601	HEM	C3B-CAB	3.74	1.55	1.47
2	C	601	HEM	C3B-CAB	3.82	1.55	1.47
2	B	601	HEM	C3B-CAB	3.83	1.55	1.47
2	D	601	HEM	C3B-CAB	3.84	1.55	1.47
2	A	601	HEM	C3C-CAC	3.90	1.55	1.47
2	C	601	HEM	C3C-CAC	3.97	1.55	1.47
2	D	601	HEM	C3C-CAC	4.01	1.55	1.47
2	B	601	HEM	C3C-CAC	4.04	1.55	1.47

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	SI5	O1-C8-C10	-3.93	103.18	108.50
3	C	602	SI5	O1-C8-C10	-3.33	104.00	108.50
3	B	602	SI5	O1-C8-C10	-3.15	104.23	108.50
3	A	602	SI5	O1-C8-C10	-2.83	104.67	108.50
2	A	601	HEM	CAA-CBA-CGA	-2.82	107.84	112.66
2	D	601	HEM	CBD-CAD-C3D	-2.61	107.48	112.47
2	B	601	HEM	CAA-CBA-CGA	-2.59	108.24	112.66
2	C	601	HEM	CAA-CBA-CGA	-2.57	108.27	112.66
2	C	601	HEM	CBD-CAD-C3D	-2.50	107.70	112.47
2	B	601	HEM	CMC-C2C-C3C	2.01	128.54	124.88
2	C	601	HEM	CMC-C2C-C3C	2.01	128.54	124.88
2	D	601	HEM	CMC-C2C-C3C	2.05	128.61	124.88
2	B	601	HEM	CMB-C2B-C3B	2.08	128.66	124.88
2	A	601	HEM	CMB-C2B-C3B	2.13	128.75	124.88
2	C	601	HEM	CMB-C2B-C3B	2.13	128.75	124.88
2	A	601	HEM	CMC-C2C-C3C	2.13	128.76	124.88
2	B	601	HEM	C4A-C3A-C2A	2.18	108.52	107.00
2	D	601	HEM	CMB-C2B-C3B	2.33	129.13	124.88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	SI5	C12-C11-N1	2.44	113.71	109.70
3	D	602	SI5	C12-C11-N1	2.51	113.83	109.70
3	A	602	SI5	C12-C11-N1	2.55	113.90	109.70
3	B	602	SI5	C12-C11-N1	2.60	113.98	109.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	4	0
3	A	602	SI5	1	0
2	B	601	HEM	6	0
3	B	602	SI5	1	0
2	C	601	HEM	6	0
2	D	601	HEM	4	0
3	D	602	SI5	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	464/479 (96%)	0.57	50 (10%) 6 5	28, 47, 101, 124	0
1	B	455/479 (94%)	0.43	31 (6%) 17 18	26, 46, 100, 115	0
1	C	446/479 (93%)	0.69	51 (11%) 5 4	29, 52, 102, 123	0
1	D	452/479 (94%)	0.73	52 (11%) 5 4	31, 55, 104, 134	0
All	All	1817/1916 (94%)	0.60	184 (10%) 7 6	26, 50, 103, 134	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	75	TRP	10.7
1	C	33	LEU	7.6
1	C	38	LEU	7.0
1	A	38	LEU	6.9
1	D	38	LEU	6.8
1	A	219	PHE	6.7
1	A	48	HIS	6.1
1	B	38	LEU	6.0
1	A	32	LYS	6.0
1	D	40	LEU	5.9
1	D	231	LEU	5.8
1	C	39	PRO	5.8
1	C	380	ARG	5.7
1	A	41	PRO	5.6
1	D	37	PRO	5.6
1	C	219	PHE	5.6
1	D	380	ARG	5.4
1	A	75	TRP	5.3
1	A	231	LEU	5.3
1	D	235	ALA	5.3
1	A	39	PRO	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	234	PRO	5.2
1	D	144	LEU	5.1
1	B	75	TRP	5.1
1	B	48	HIS	5.1
1	C	65	PHE	5.0
1	D	39	PRO	4.9
1	D	65	PHE	4.7
1	C	75	TRP	4.6
1	D	219	PHE	4.6
1	A	40	LEU	4.5
1	C	231	LEU	4.5
1	A	47	LEU	4.4
1	D	423	ALA	4.4
1	D	33	LEU	4.4
1	C	238	GLY	4.3
1	A	33	LEU	4.3
1	B	33	LEU	4.2
1	C	55	PRO	4.2
1	D	471	GLY	4.2
1	C	56	TYR	4.2
1	A	229	VAL	4.2
1	D	240	VAL	4.1
1	D	234	PRO	4.1
1	C	424	GLN	4.0
1	D	220	LEU	3.9
1	C	236	LEU	3.8
1	C	36	GLY	3.8
1	C	228	PRO	3.8
1	A	342	VAL	3.8
1	C	168	SER	3.8
1	A	223	VAL	3.7
1	A	228	PRO	3.7
1	D	64	ARG	3.7
1	B	240	VAL	3.7
1	C	229	VAL	3.7
1	D	424	GLN	3.6
1	A	483	PHE	3.6
1	B	237	ALA	3.6
1	C	240	VAL	3.6
1	A	217	SER	3.6
1	A	56	TYR	3.6
1	A	144	LEU	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	306	GLY	3.5
1	B	231	LEU	3.4
1	B	236	LEU	3.4
1	A	145	GLY	3.4
1	A	234	PRO	3.4
1	B	32	LYS	3.4
1	C	306	GLY	3.4
1	C	310	THR	3.4
1	C	64	ARG	3.4
1	B	307	MET	3.3
1	B	234	PRO	3.3
1	B	235	ALA	3.2
1	C	481	PHE	3.2
1	A	37	PRO	3.2
1	A	232	HIS	3.2
1	D	333	GLN	3.2
1	A	149	LEU	3.2
1	B	149	LEU	3.2
1	D	389	ILE	3.2
1	D	238	GLY	3.1
1	D	483	PHE	3.1
1	D	305	ALA	3.1
1	B	39	PRO	3.1
1	C	37	PRO	3.1
1	B	310	THR	3.0
1	D	151	GLN	3.0
1	B	309	THR	3.0
1	D	229	VAL	3.0
1	C	342	VAL	3.0
1	B	305	ALA	2.9
1	A	143	GLY	2.9
1	B	306	GLY	2.9
1	D	55	PRO	2.9
1	D	381	ASP	2.9
1	D	239	LYS	2.9
1	C	343	ARG	2.9
1	B	380	ARG	2.8
1	A	43	LEU	2.8
1	C	369	ILE	2.8
1	C	389	ILE	2.8
1	C	423	ALA	2.8
1	C	60	GLN	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	310	THR	2.8
1	A	240	VAL	2.7
1	C	224	LEU	2.7
1	D	236	LEU	2.7
1	A	49	VAL	2.7
1	A	309	THR	2.7
1	D	314	LEU	2.7
1	C	35	PRO	2.7
1	C	425	GLY	2.7
1	C	313	THR	2.7
1	A	235	ALA	2.7
1	B	219	PHE	2.6
1	D	36	GLY	2.6
1	D	60	GLN	2.6
1	C	223	VAL	2.6
1	B	342	VAL	2.6
1	D	310	THR	2.6
1	A	303	PHE	2.6
1	A	307	MET	2.6
1	D	313	THR	2.5
1	D	56	TYR	2.5
1	B	64	ARG	2.5
1	A	238	GLY	2.5
1	B	238	GLY	2.5
1	C	218	GLY	2.5
1	D	383	GLU	2.5
1	C	235	ALA	2.5
1	D	76	THR	2.5
1	D	309	THR	2.5
1	B	45	ASN	2.5
1	D	306	GLY	2.5
1	C	63	ARG	2.4
1	C	309	THR	2.4
1	C	96	GLU	2.4
1	D	61	LEU	2.4
1	A	369	ILE	2.4
1	C	339	ILE	2.4
1	C	237	ALA	2.4
1	A	227	VAL	2.3
1	B	228	PRO	2.3
1	D	307	MET	2.3
1	A	242	ARG	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	72	GLN	2.3
1	B	148	SER	2.3
1	C	109	ILE	2.3
1	D	312	THR	2.3
1	C	307	MET	2.2
1	B	303	PHE	2.2
1	B	218	GLY	2.2
1	D	147	LYS	2.2
1	A	343	ARG	2.2
1	C	484	LEU	2.2
1	A	312	THR	2.2
1	B	369	ILE	2.2
1	A	340	GLY	2.2
1	D	35	PRO	2.2
1	D	133	ARG	2.2
1	A	96	GLU	2.2
1	A	233	ILE	2.1
1	D	69	PHE	2.1
1	A	314	LEU	2.1
1	D	146	LYS	2.1
1	D	481	PHE	2.1
1	A	308	VAL	2.1
1	C	471	GLY	2.1
1	A	237	ALA	2.1
1	C	227	VAL	2.1
1	A	313	THR	2.1
1	D	303	PHE	2.1
1	C	54	THR	2.1
1	B	229	VAL	2.1
1	C	384	VAL	2.1
1	D	390	PRO	2.1
1	A	304	SER	2.1
1	B	49	VAL	2.0
1	A	146	LYS	2.0
1	A	147	LYS	2.0
1	C	390	PRO	2.0
1	D	472	GLN	2.0

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

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

### 6.3 Carbohydrates [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( $\text{\AA}^2$ )	Q<0.9
4	ZN	C	607	1/1	0.39	0.09	122,122,122,122	0
3	SI5	A	602	25/25	0.81	0.27	47,76,88,89	0
4	ZN	D	607	1/1	0.82	0.07	130,130,130,130	0
3	SI5	B	602	25/25	0.87	0.23	39,71,78,86	0
4	ZN	B	605	1/1	0.88	0.10	76,76,76,76	0
3	SI5	D	602	25/25	0.89	0.18	48,75,84,85	0
3	SI5	C	602	25/25	0.89	0.22	48,72,82,85	0
4	ZN	C	606	1/1	0.89	0.06	79,79,79,79	0
4	ZN	C	605	1/1	0.90	0.08	89,89,89,89	0
4	ZN	D	605	1/1	0.91	0.08	84,84,84,84	0
4	ZN	A	604	1/1	0.93	0.23	69,69,69,69	0
4	ZN	D	606	1/1	0.94	0.07	92,92,92,92	0
4	ZN	D	604	1/1	0.95	0.18	72,72,72,72	0
4	ZN	A	605	1/1	0.95	0.06	75,75,75,75	0
4	ZN	C	604	1/1	0.95	0.13	69,69,69,69	0
4	ZN	B	604	1/1	0.96	0.20	70,70,70,70	0
2	HEM	A	601	43/43	0.97	0.24	18,28,37,39	0
2	HEM	D	601	43/43	0.97	0.20	23,38,47,52	0
2	HEM	C	601	43/43	0.98	0.23	25,36,44,46	0
2	HEM	B	601	43/43	0.98	0.24	19,31,37,43	0
4	ZN	B	603	1/1	0.99	0.16	36,36,36,36	0
4	ZN	A	606	1/1	0.99	0.10	46,46,46,46	0
4	ZN	A	603	1/1	0.99	0.16	33,33,33,33	0
4	ZN	C	603	1/1	0.99	0.16	37,37,37,37	0
4	ZN	D	603	1/1	0.99	0.13	39,39,39,39	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.