



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:57 pm GMT

PDB ID : 1WVE  
Title : p-Cresol Methylhydroxylase: Alteration of the Structure of the Flavoprotein Subunit upon its Binding to the Cytochrome Subunit  
Authors : Cunane, L.M.; Chen, Z.-W.; McIntire, W.S.; Mathews, F.S.  
Deposited on : 2004-12-15  
Resolution : 1.85 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.

---

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

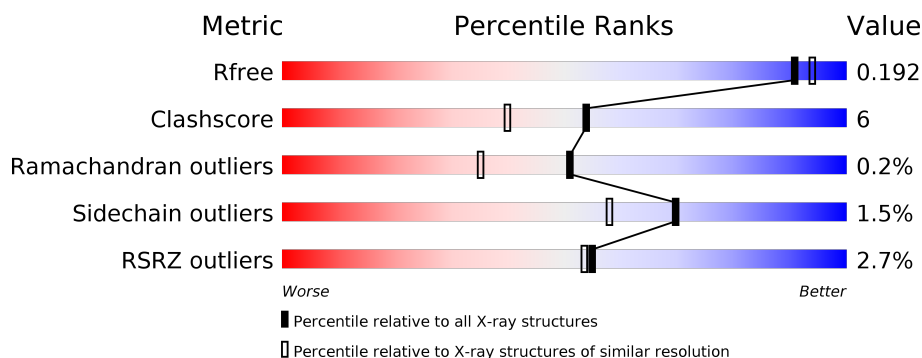
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1923 (1.86-1.86)
Clashscore	112137	2083 (1.86-1.86)
Ramachandran outliers	110173	2060 (1.86-1.86)
Sidechain outliers	110143	2060 (1.86-1.86)
RSRZ outliers	101464	1932 (1.86-1.86)

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	520	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>•</div> </div> </div>
1	B	520	<div> <div>3%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>••</div> </div> </div>
2	C	80	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>••</div> <div>6%</div> </div> </div>
2	D	80	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>10%</div> <div>•</div> <div>6%</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
5	TRS	A	2705	-	-	-	X
5	TRS	B	1705	-	-	-	X
5	TRS	B	2704	-	-	-	X
7	ACY	A	1701	-	-	-	X
7	ACY	A	2701	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10692 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 4-cresol dehydrogenase [hydroxylating] flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	515	Total	C	N	O	S	0	7	0
			4082	2596	696	760	30			
1	B	515	Total	C	N	O	S	0	11	0
			4123	2619	705	767	32			

- Molecule 2 is a protein called 4-cresol dehydrogenase [hydroxylating] cytochrome c subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	75	Total	C	N	O	S	0	0	0
			571	363	97	108	3			
2	D	75	Total	C	N	O	S	0	0	0
			571	363	97	108	3			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

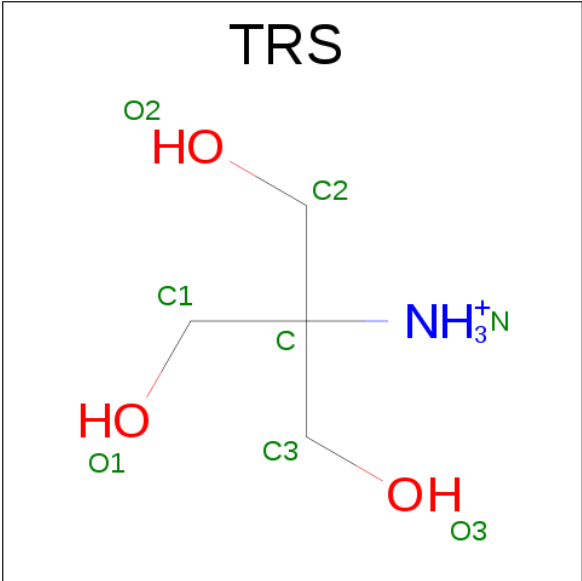
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



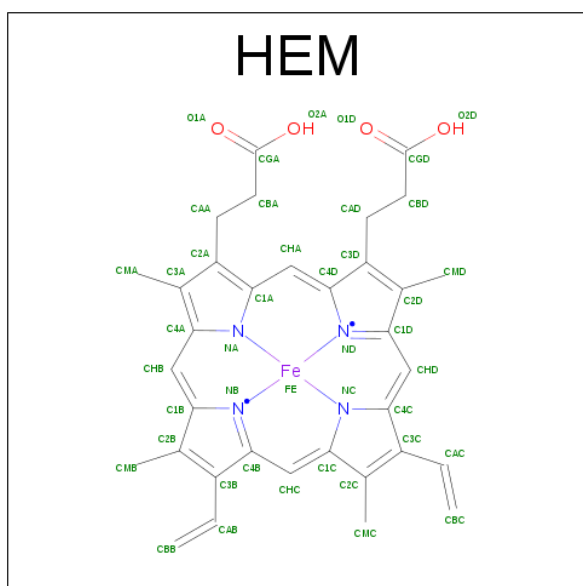
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

Continued on next page...

Continued from previous page...

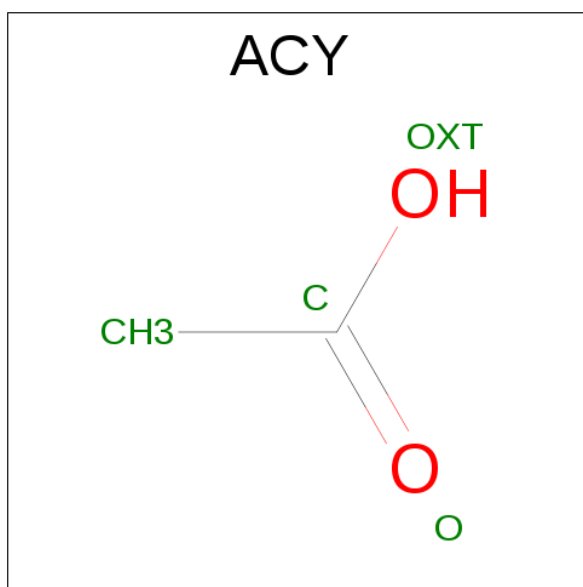
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	B	1	Total	C	N	O	0	0
			8	4	1	3		
5	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula:  $C_2H_4O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

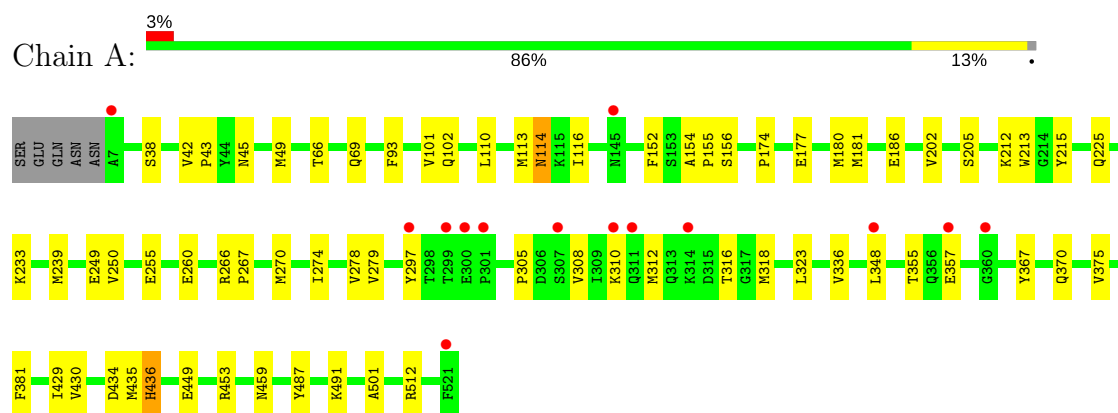
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	499	Total	O	0	0
			499	499		
8	B	441	Total	O	0	0
			441	441		
8	C	83	Total	O	0	0
			83	83		
8	D	80	Total	O	0	0
			80	80		

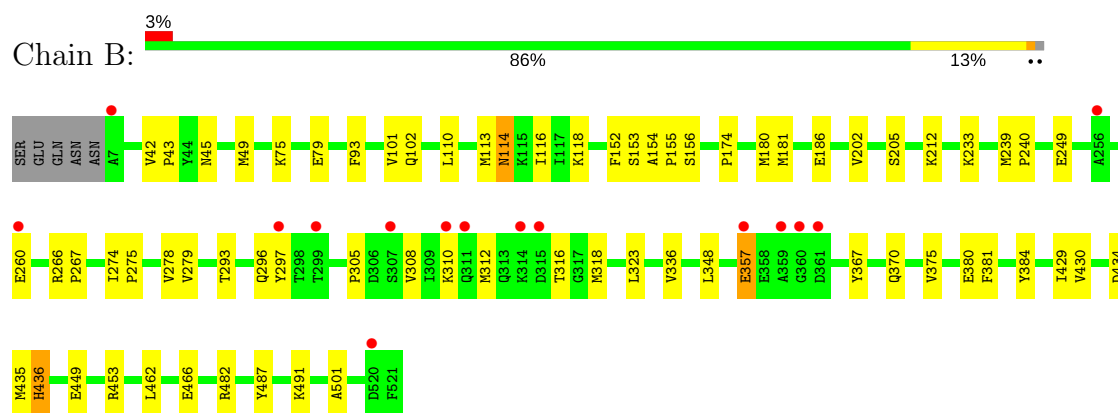
### 3 Residue-property plots [i](#)

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.

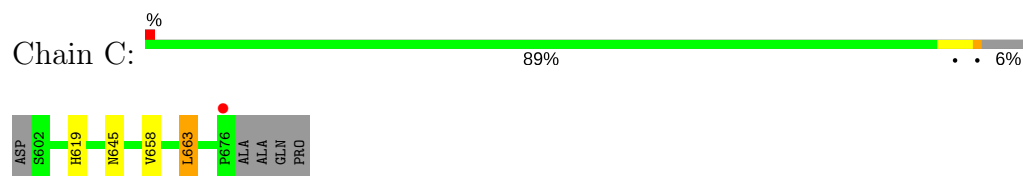
- Molecule 1: 4-cresol dehydrogenase [hydroxylating] flavoprotein subunit



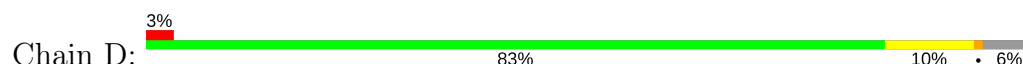
- Molecule 1: 4-cresol dehydrogenase [hydroxylating] flavoprotein subunit



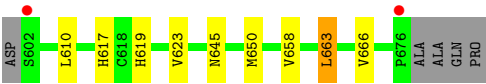
- Molecule 2: 4-cresol dehydrogenase [hydroxylating] cytochrome c subunit



- Molecule 2: 4-cresol dehydrogenase [hydroxylating] cytochrome c subunit







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.83Å 118.60Å 136.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 28.47 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.7 (30.00-1.85) 87.3 (28.47-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 1.80Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.159 , 0.194 0.159 , 0.192	Depositor DCC
$R_{free}$ test set	9407 reflections (11.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 57.1	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	0.97	EDS
Total number of atoms	10692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, TRS, ACY, FAD, CL

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	0.42	0/4180	0.67	3/5669 (0.1%)
1	B	0.43	0/4221	0.66	3/5720 (0.1%)
2	C	0.43	0/587	0.70	1/798 (0.1%)
2	D	0.44	0/587	0.70	1/798 (0.1%)
All	All	0.43	0/9575	0.67	8/12985 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	619	HIS	ND1-CG-CD2	7.88	119.84	108.80
2	C	619	HIS	ND1-CG-CD2	7.86	119.81	108.80
1	B	436	HIS	N-CA-C	-6.34	93.89	111.00
1	A	436	HIS	N-CA-C	-6.29	94.03	111.00
1	A	116	ILE	N-CA-C	-5.44	96.32	111.00
1	B	274	ILE	N-CA-C	-5.34	96.59	111.00
1	B	116	ILE	N-CA-C	-5.32	96.62	111.00
1	A	274	ILE	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	384	TYR	Sidechain

## 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	4082	0	4007	56	0
1	B	4123	0	4044	54	0
2	C	571	0	550	3	0
2	D	571	0	550	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	28	2	0
4	B	53	0	28	3	0
5	A	16	0	24	0	0
5	B	16	0	24	0	0
6	C	43	0	30	1	0
6	D	43	0	30	2	0
7	A	12	0	9	2	0
7	B	4	0	3	1	0
8	A	499	0	0	10	0
8	B	441	0	0	6	0
8	C	83	0	0	0	0
8	D	80	0	0	0	0
All	All	10692	0	9327	116	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 6.

All (116) 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:174:PRO:HB2	1:A:239:MET:HE3	1.60	0.83
1:A:212:LYS:NZ	8:A:3162:HOH:O	2.23	0.69
1:B:42:VAL:HG13	1:B:43:PRO:HD3	1.74	0.69
1:A:355:THR:HB	1:A:357:GLU:OE2	1.92	0.69
1:A:357:GLU:CD	1:A:357:GLU:H	1.97	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:HB2	1:B:239[A]:MET:HE3	1.75	0.69
1:A:266:ARG:HB3	1:A:267:PRO:HD3	1.76	0.67
1:A:501:ALA:HB2	1:B:501:ALA:HB2	1.78	0.66
1:A:154:ALA:HB2	8:A:3190:HOH:O	1.98	0.64
1:B:118:LYS:HE2	8:B:3103:HOH:O	1.98	0.63
1:A:180[A]:MET:HG2	1:A:181:MET:HE2	1.80	0.63
1:B:180[A]:MET:HG2	1:B:181:MET:HE2	1.81	0.62
1:A:180[B]:MET:HG3	8:A:3056:HOH:O	1.99	0.62
1:B:212:LYS:NZ	8:B:3088:HOH:O	2.30	0.61
1:A:38:SER:O	1:A:42[B]:VAL:HG23	2.02	0.59
1:B:462:LEU:O	1:B:466[B]:GLU:HG3	2.03	0.58
1:A:174:PRO:HB2	1:A:239:MET:CE	2.34	0.58
1:B:174:PRO:HB2	1:B:239[A]:MET:CE	2.34	0.57
1:B:357:GLU:H	1:B:357:GLU:CD	2.08	0.57
1:B:266:ARG:HB3	1:B:267:PRO:HD3	1.87	0.55
1:B:180[A]:MET:HG2	1:B:181:MET:CE	2.37	0.55
1:B:381:PHE:CD1	6:D:699:HEM:HBC1	2.43	0.54
1:A:180[A]:MET:HG2	1:A:181:MET:CE	2.38	0.53
8:A:3056:HOH:O	1:B:180[B]:MET:HG3	2.08	0.53
1:A:93:PHE:HB2	4:A:599:FAD:HM81	1.90	0.53
1:B:430:VAL:HG22	1:B:435:MET:SD	2.49	0.53
1:B:93:PHE:HB2	4:B:599:FAD:HM81	1.91	0.53
1:B:75:LYS:O	1:B:79[A]:GLU:HG3	2.10	0.52
1:A:260[A]:GLU:HB3	1:A:348:LEU:HD11	1.93	0.51
1:B:153:SER:HB2	1:B:155:PRO:HD2	1.92	0.51
1:B:42:VAL:HG13	1:B:43:PRO:CD	2.40	0.51
1:A:355:THR:OG1	1:A:357:GLU:HG2	2.11	0.51
1:A:110:LEU:HD13	1:A:113[B]:MET:HE1	1.91	0.51
1:A:186:GLU:HB3	1:A:233:LYS:HB2	1.93	0.51
2:C:658:VAL:HG12	2:C:663:LEU:HD13	1.93	0.51
1:B:466[B]:GLU:CD	1:B:482:ARG:HH22	2.13	0.51
1:A:336:VAL:HG21	1:B:336:VAL:HG21	1.92	0.50
1:B:316:THR:OG1	1:B:318:MET:HG3	2.11	0.50
1:B:305:PRO:HB2	1:B:308:VAL:HG23	1.94	0.50
1:A:370:GLN:HB3	1:A:375:VAL:HB	1.93	0.49
8:A:2818:HOH:O	1:B:491:LYS:HE3	2.11	0.49
2:D:658:VAL:HG12	2:D:663:LEU:HD13	1.93	0.49
1:A:316:THR:OG1	1:A:318:MET:HG3	2.12	0.49
1:B:293:THR:OG1	1:B:296:GLN:HG3	2.13	0.49
1:B:487:TYR:HB3	1:B:491:LYS:HD3	1.95	0.48
1:B:101:VAL:HG13	1:B:102:GLN:HG3	1.95	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ILE:HB	1:B:436:HIS:HB2	1.95	0.48
1:A:202:VAL:HB	1:A:205:SER:HB2	1.94	0.48
7:B:1702:ACY:H1	8:B:3130:HOH:O	2.12	0.48
1:B:449:GLU:OE2	1:B:453:ARG:NE	2.37	0.48
1:A:381:PHE:CD1	6:C:699:HEM:HBC1	2.49	0.48
2:D:650:MET:HB2	6:D:699:HEM:C1D	2.49	0.47
1:A:491:LYS:HE3	8:B:2831:HOH:O	2.13	0.47
4:A:599:FAD:H8A	4:A:599:FAD:O5B	2.14	0.47
1:B:202:VAL:HB	1:B:205:SER:HB2	1.97	0.47
1:A:110:LEU:HD13	1:A:113[B]:MET:CE	2.44	0.47
1:A:212:LYS:HE3	1:A:213:TRP:CZ3	2.49	0.47
1:A:323:LEU:HD23	1:A:323:LEU:C	2.35	0.46
1:A:429:ILE:HB	1:A:436:HIS:HB2	1.98	0.46
1:A:225:GLN:HA	1:A:512:ARG:NH2	2.29	0.46
1:A:42[B]:VAL:HG11	2:C:645:ASN:OD1	2.15	0.46
1:B:186:GLU:HB3	1:B:233:LYS:HB2	1.96	0.46
1:B:42:VAL:CG1	1:B:43:PRO:HD3	2.45	0.46
1:A:297:TYR:CE2	1:A:312:MET:HG2	2.50	0.46
1:A:310:LYS:NZ	1:A:310:LYS:HB3	2.31	0.46
1:A:430:VAL:HG22	1:A:435:MET:SD	2.55	0.45
1:A:249:GLU:HG2	1:A:250:VAL:N	2.32	0.45
1:A:487:TYR:HB3	1:A:491:LYS:HD3	1.98	0.45
1:B:310:LYS:HB3	1:B:310:LYS:NZ	2.30	0.45
1:A:278:VAL:HG12	1:A:279:VAL:N	2.30	0.45
4:B:599:FAD:O5B	4:B:599:FAD:H8A	2.16	0.45
1:A:336:VAL:CG2	1:B:336:VAL:HG21	2.46	0.45
1:A:305:PRO:HB2	1:A:308:VAL:HG23	1.99	0.45
1:A:42[A]:VAL:CG1	1:A:43:PRO:HD3	2.46	0.45
1:B:449:GLU:HG2	8:B:3067:HOH:O	2.17	0.44
1:B:278:VAL:HG12	1:B:279:VAL:N	2.32	0.44
1:A:260[B]:GLU:HB3	1:A:348:LEU:HD11	2.00	0.44
1:B:154:ALA:N	1:B:155:PRO:CD	2.81	0.44
1:A:449:GLU:OE2	1:A:453:ARG:NE	2.33	0.43
1:A:42[A]:VAL:HG13	1:A:43:PRO:HD3	2.00	0.43
1:B:323:LEU:C	1:B:323:LEU:HD23	2.38	0.43
1:B:110:LEU:HD13	1:B:113[B]:MET:HE1	2.00	0.43
1:B:42:VAL:HG21	2:D:645:ASN:OD1	2.19	0.43
2:D:658:VAL:CG1	2:D:663:LEU:HD13	2.49	0.43
1:A:66:THR:OG1	1:A:69:GLN:HG3	2.19	0.42
1:A:215:TYR:HB3	1:B:487:TYR:CE2	2.54	0.42
1:A:255:GLU:HG3	8:A:3067:HOH:O	2.18	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLU:HB3	1:B:348:LEU:HD11	2.01	0.42
7:A:2701:ACY:H2	8:A:3201:HOH:O	2.18	0.42
1:A:114:ASN:N	1:A:114:ASN:HD22	2.16	0.42
1:B:297:TYR:CE2	1:B:312:MET:HG2	2.54	0.42
1:B:249:GLU:HA	1:B:323:LEU:O	2.19	0.42
2:C:663:LEU:HD12	2:C:663:LEU:HA	1.88	0.42
1:A:459[B]:ASN:ND2	8:A:2837:HOH:O	2.39	0.41
1:B:153:SER:CB	1:B:155:PRO:HD2	2.50	0.41
2:D:663:LEU:HD12	2:D:663:LEU:HA	1.87	0.41
2:D:617:HIS:O	2:D:623:VAL:HG11	2.20	0.41
1:A:270:MET:CG	1:B:240:PRO:HG2	2.51	0.41
1:B:49:MET:HG2	8:B:2822:HOH:O	2.19	0.41
1:A:154:ALA:N	1:A:155:PRO:CD	2.83	0.41
1:A:278:VAL:CG1	1:A:279:VAL:N	2.84	0.41
1:A:49:MET:HG2	8:A:2846:HOH:O	2.21	0.41
1:B:174:PRO:HG2	1:B:239[A]:MET:HE1	2.02	0.41
1:B:380:GLU:OE2	4:B:599:FAD:H6	2.21	0.41
2:D:610:LEU:HD23	2:D:666:VAL:HB	2.01	0.41
1:A:279:VAL:O	1:A:323:LEU:HA	2.20	0.40
1:B:278:VAL:CG1	1:B:279:VAL:N	2.84	0.40
1:A:101:VAL:HG13	1:A:102:GLN:HG3	2.03	0.40
7:A:1701:ACY:H1	8:A:3184:HOH:O	2.21	0.40
1:A:270:MET:HG2	1:B:240:PRO:CG	2.51	0.40
1:A:336:VAL:HG21	1:B:336:VAL:CG2	2.51	0.40
1:B:370:GLN:HB3	1:B:375:VAL:HB	2.03	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	520/520 (100%)	510 (98%)	9 (2%)	1 (0%)	51 35

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	524/520 (101%)	514 (98%)	9 (2%)	1 (0%)	51	35
2	C	73/80 (91%)	69 (94%)	4 (6%)	0	100	100
2	D	73/80 (91%)	71 (97%)	2 (3%)	0	100	100
All	All	1190/1200 (99%)	1164 (98%)	24 (2%)	2 (0%)	51	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	SER
1	B	156	SER

### 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	434/432 (100%)	427 (98%)	7 (2%)	68	55
1	B	438/432 (101%)	431 (98%)	7 (2%)	68	55
2	C	61/64 (95%)	60 (98%)	1 (2%)	68	55
2	D	61/64 (95%)	60 (98%)	1 (2%)	68	55
All	All	994/992 (100%)	978 (98%)	16 (2%)	70	55

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	114	ASN
1	A	152	PHE
1	A	177[A]	GLU
1	A	177[B]	GLU
1	A	367	TYR
1	A	434	ASP
2	C	663	LEU
1	B	45	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	114	ASN
1	B	152	PHE
1	B	275	PRO
1	B	357	GLU
1	B	367	TYR
1	B	434	ASP
2	D	663	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	19	ASN
1	A	114	ASN
1	A	272	ASN
1	A	311	GLN
1	A	313	GLN
1	A	518	ASN
1	B	15	GLN
1	B	19	ASN
1	B	114	ASN
1	B	311	GLN
1	B	313	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 14 ligands modelled in this entry, 2 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$
7	ACY	A	1701	-	1,3,3	2.82	1 (100%)	0,3,3	0.00	-
5	TRS	A	1704	-	7,7,7	0.61	0	9,9,9	1.56	3 (33%)
7	ACY	A	2701	-	1,3,3	3.43	1 (100%)	0,3,3	0.00	-
7	ACY	A	2702	-	1,3,3	2.78	1 (100%)	0,3,3	0.00	-
5	TRS	A	2705	-	7,7,7	0.71	0	9,9,9	1.73	3 (33%)
4	FAD	A	599	1	51,58,58	2.50	18 (35%)	54,89,89	3.07	17 (31%)
7	ACY	B	1702	-	1,3,3	2.19	1 (100%)	0,3,3	0.00	-
5	TRS	B	1705	-	7,7,7	0.61	0	9,9,9	1.54	3 (33%)
5	TRS	B	2704	-	7,7,7	0.66	0	9,9,9	1.59	3 (33%)
4	FAD	B	599	1	51,58,58	2.41	16 (31%)	54,89,89	3.14	18 (33%)
6	HEM	C	699	2	28,50,50	2.01	9 (32%)	17,82,82	1.58	4 (23%)
6	HEM	D	699	2	28,50,50	1.97	8 (28%)	17,82,82	1.59	5 (29%)

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
7	ACY	A	1701	-	-	0/0/0/0	0/0/0/0
5	TRS	A	1704	-	-	0/9/9/9	0/0/0/0
7	ACY	A	2701	-	-	0/0/0/0	0/0/0/0
7	ACY	A	2702	-	-	0/0/0/0	0/0/0/0
5	TRS	A	2705	-	-	0/9/9/9	0/0/0/0
4	FAD	A	599	1	-	0/28/50/50	0/6/6/6
7	ACY	B	1702	-	-	0/0/0/0	0/0/0/0
5	TRS	B	1705	-	-	0/9/9/9	0/0/0/0
5	TRS	B	2704	-	-	0/9/9/9	0/0/0/0
4	FAD	B	599	1	-	0/28/50/50	0/6/6/6
6	HEM	C	699	2	-	0/6/54/54	0/0/8/8
6	HEM	D	699	2	-	0/6/54/54	0/0/8/8

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	599	FAD	O2'-C2'	-4.77	1.32	1.43
6	C	699	HEM	C3C-C2C	-4.75	1.34	1.40
4	A	599	FAD	C8A-N7A	-4.40	1.26	1.34
4	B	599	FAD	C8M-C8	-4.29	1.42	1.51
6	D	699	HEM	C3C-C2C	-4.21	1.34	1.40
4	A	599	FAD	C8M-C8	-4.07	1.43	1.51
4	B	599	FAD	O2'-C2'	-4.04	1.34	1.43
4	B	599	FAD	C8A-N7A	-3.84	1.27	1.34
4	B	599	FAD	O3'-C3'	-3.37	1.35	1.43
4	A	599	FAD	O3'-C3'	-3.05	1.35	1.43
6	C	699	HEM	C3B-C2B	-2.84	1.36	1.40
6	D	699	HEM	C3B-C2B	-2.58	1.36	1.40
4	A	599	FAD	C4'-C3'	2.06	1.57	1.53
6	C	699	HEM	CMC-C2C	2.11	1.56	1.51
4	A	599	FAD	C2A-N1A	2.14	1.37	1.33
7	B	1702	ACY	CH3-C	2.19	1.51	1.48
6	C	699	HEM	CMD-C2D	2.25	1.56	1.51
6	D	699	HEM	C1D-ND	2.27	1.41	1.36
6	D	699	HEM	C4D-ND	2.32	1.39	1.36
6	C	699	HEM	C3B-CAB	2.40	1.52	1.47
4	B	599	FAD	C9A-C5X	2.50	1.47	1.42
4	A	599	FAD	C9A-C5X	2.50	1.47	1.42
4	B	599	FAD	C6-C5X	2.65	1.45	1.41
6	C	699	HEM	C3C-CAC	2.73	1.53	1.47
7	A	2702	ACY	CH3-C	2.78	1.52	1.48
7	A	1701	ACY	CH3-C	2.82	1.52	1.48
4	A	599	FAD	C8-C7	2.91	1.48	1.41
6	C	699	HEM	C1B-NB	2.93	1.40	1.36
4	A	599	FAD	C6-C5X	2.93	1.46	1.41
6	D	699	HEM	C3C-CAC	3.01	1.53	1.47
4	B	599	FAD	C8-C7	3.07	1.48	1.41
4	B	599	FAD	C2'-C3'	3.29	1.60	1.53
6	D	699	HEM	C3B-CAB	3.41	1.54	1.47
7	A	2701	ACY	CH3-C	3.43	1.53	1.48
6	D	699	HEM	CBB-CAB	3.60	1.54	1.28
4	A	599	FAD	O4B-C1B	3.71	1.46	1.41
4	B	599	FAD	C2A-N3A	3.71	1.38	1.32
6	C	699	HEM	CBC-CAC	3.74	1.55	1.28
4	A	599	FAD	C2'-C3'	3.76	1.60	1.53
6	D	699	HEM	CBC-CAC	3.77	1.55	1.28
4	A	599	FAD	C2A-N3A	3.77	1.38	1.32
6	C	699	HEM	CBB-CAB	3.85	1.56	1.28

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	599	FAD	O4B-C1B	4.03	1.46	1.41
4	A	599	FAD	C4X-N5	4.10	1.39	1.33
4	B	599	FAD	C4A-N3A	4.12	1.41	1.35
4	A	599	FAD	C10-N1	4.16	1.39	1.33
4	A	599	FAD	C1'-N10	4.18	1.52	1.48
4	B	599	FAD	C4X-N5	4.28	1.39	1.33
4	A	599	FAD	C4A-N3A	4.29	1.41	1.35
4	B	599	FAD	C10-N1	4.35	1.39	1.33
4	B	599	FAD	C1'-N10	4.39	1.52	1.48
4	B	599	FAD	C4-N3	5.27	1.42	1.33
4	A	599	FAD	C4-N3	5.75	1.43	1.33
4	B	599	FAD	C9A-N10	6.48	1.47	1.38
4	A	599	FAD	C9A-N10	7.07	1.48	1.38

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	599	FAD	C4X-C10-N10	-6.76	115.83	120.52
4	B	599	FAD	C4X-C10-N10	-6.64	115.91	120.52
4	B	599	FAD	C4X-C4-N3	-5.15	116.15	123.48
4	A	599	FAD	C4X-C4-N3	-5.10	116.22	123.48
4	B	599	FAD	C4-C4X-C10	-5.09	115.84	119.96
4	A	599	FAD	C4-C4X-C10	-4.65	116.20	119.96
4	B	599	FAD	O5'-C5'-C4'	-4.43	97.55	109.36
4	A	599	FAD	O5'-C5'-C4'	-4.39	97.64	109.36
4	B	599	FAD	O4'-C4'-C3'	-3.69	99.94	109.09
4	A	599	FAD	O4'-C4'-C3'	-3.56	100.26	109.09
4	A	599	FAD	C4-C4X-N5	-3.55	114.79	118.68
4	B	599	FAD	C4-C4X-N5	-3.07	115.31	118.68
4	A	599	FAD	C6-C5X-N5	-3.01	115.44	118.97
4	A	599	FAD	C4X-N5-C5X	-2.96	113.63	116.76
4	B	599	FAD	C6-C5X-N5	-2.83	115.64	118.97
4	B	599	FAD	C4X-N5-C5X	-2.81	113.80	116.76
6	C	699	HEM	CMD-C2D-C1D	-2.61	124.45	128.46
6	C	699	HEM	CMA-C3A-C4A	-2.57	124.52	128.46
4	B	599	FAD	N3A-C2A-N1A	-2.54	126.64	128.86
4	B	599	FAD	C8M-C8-C9	-2.53	113.99	120.34
6	D	699	HEM	CBA-CAA-C2A	-2.49	107.72	112.48
4	B	599	FAD	O3'-C3'-C2'	-2.46	102.71	108.82
4	A	599	FAD	C8M-C8-C9	-2.45	114.19	120.34
4	A	599	FAD	O3'-C3'-C2'	-2.44	102.78	108.82
6	D	699	HEM	CMD-C2D-C1D	-2.40	124.78	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	699	HEM	CMA-C3A-C4A	-2.38	124.80	128.46
6	C	699	HEM	CBD-CAD-C3D	-2.34	108.00	112.47
4	A	599	FAD	N3A-C2A-N1A	-2.19	126.95	128.86
6	D	699	HEM	CMB-C2B-C3B	2.06	128.72	124.89
4	B	599	FAD	O2'-C2'-C3'	2.11	114.33	109.09
4	B	599	FAD	C9A-C5X-N5	2.26	125.60	122.24
4	A	599	FAD	C9A-C5X-N5	2.30	125.67	122.24
5	B	2704	TRS	O3-C3-C	2.37	117.32	110.47
5	B	1705	TRS	O2-C2-C	2.38	117.37	110.47
5	A	1704	TRS	O1-C1-C	2.41	117.45	110.47
5	B	1705	TRS	O1-C1-C	2.45	117.57	110.47
6	C	699	HEM	CMC-C2C-C3C	2.49	129.51	124.89
5	A	1704	TRS	O3-C3-C	2.50	117.69	110.47
5	B	1705	TRS	O3-C3-C	2.50	117.72	110.47
5	A	2705	TRS	O3-C3-C	2.53	117.80	110.47
5	A	1704	TRS	O2-C2-C	2.54	117.81	110.47
5	B	2704	TRS	O1-C1-C	2.58	117.94	110.47
5	B	2704	TRS	O2-C2-C	2.66	118.17	110.47
5	A	2705	TRS	O2-C2-C	2.73	118.36	110.47
6	D	699	HEM	CMC-C2C-C3C	2.80	130.09	124.89
5	A	2705	TRS	O1-C1-C	3.11	119.48	110.47
4	B	599	FAD	C1'-N10-C9A	3.67	121.71	118.35
4	A	599	FAD	C1'-C2'-C3'	4.13	121.64	109.82
4	A	599	FAD	C1'-N10-C9A	4.15	122.15	118.35
4	B	599	FAD	C1'-C2'-C3'	4.31	122.14	109.82
4	A	599	FAD	O4'-C4'-C5'	4.48	119.99	110.00
4	B	599	FAD	O4'-C4'-C5'	4.94	121.01	110.00
4	B	599	FAD	C10-C4X-N5	6.99	128.64	120.59
4	A	599	FAD	C10-C4X-N5	7.27	128.95	120.59
4	A	599	FAD	C4-N3-C2	13.90	127.31	115.16
4	B	599	FAD	C4-N3-C2	14.64	127.97	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1701	ACY	1	0
7	A	2701	ACY	1	0
4	A	599	FAD	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1702	ACY	1	0
4	B	599	FAD	3	0
6	C	699	HEM	1	0
6	D	699	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	515/520 (99%)	-0.20	14 (2%) 55 53	11, 19, 39, 52	0
1	B	515/520 (99%)	-0.17	15 (2%) 52 50	11, 19, 39, 53	0
2	C	75/80 (93%)	-0.33	1 (1%) 77 78	14, 21, 32, 50	0
2	D	75/80 (93%)	-0.23	2 (2%) 55 53	16, 22, 32, 51	0
All	All	1180/1200 (98%)	-0.20	32 (2%) 55 53	11, 19, 39, 53	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	310	LYS	4.8
1	A	314	LYS	4.7
1	A	7	ALA	4.5
1	B	314	LYS	4.1
1	A	145	ASN	3.8
1	B	256	ALA	3.7
1	A	300	GLU	3.6
1	A	299	THR	3.6
1	A	310	LYS	3.4
1	B	361	ASP	3.4
1	B	315	ASP	3.1
1	A	297	TYR	3.1
1	B	7	ALA	3.0
1	A	348	LEU	2.9
2	C	676	PRO	2.9
1	A	311	GLN	2.8
1	A	357	GLU	2.8
2	D	676	PRO	2.7
1	B	360	GLY	2.7
1	B	299	THR	2.6
1	B	520	ASP	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	307	SER	2.5
1	A	521	PHE	2.5
1	B	357	GLU	2.5
1	B	359	ALA	2.4
1	B	307	SER	2.3
1	B	311	GLN	2.3
1	A	360	GLY	2.3
1	B	297	TYR	2.2
1	B	260	GLU	2.2
1	A	301	PRO	2.1
2	D	602	SER	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
7	ACY	A	2701	4/4	0.64	0.28	22.35	47,47,48,48	0
5	TRS	B	2704	8/8	0.93	0.21	9.32	18,30,35,35	0
5	TRS	A	2705	8/8	0.80	0.23	9.30	29,34,36,38	0
5	TRS	B	1705	8/8	0.83	0.20	3.77	25,33,35,36	0
7	ACY	A	1701	4/4	0.85	0.16	2.10	28,28,30,34	0
7	ACY	B	1702	4/4	0.91	0.14	1.34	31,31,33,33	0
3	CL	A	2703	1/1	1.00	0.09	1.26	17,17,17,17	0
5	TRS	A	1704	8/8	0.92	0.11	0.48	30,31,31,31	0
6	HEM	C	699	43/43	0.97	0.08	-0.32	11,15,23,27	0
4	FAD	B	599	53/53	0.98	0.09	-0.40	11,14,21,27	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	HEM	D	699	43/43	0.97	0.07	-0.48	13,16,22,26	0
4	FAD	A	599	53/53	0.98	0.08	-0.57	8,14,20,26	0
3	CL	B	1703	1/1	1.00	0.07	-0.94	15,15,15,15	0
7	ACY	A	2702	4/4	0.85	0.19	-	50,51,51,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.