



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 11:37 PM GMT

PDB ID : 1CCK
Title : ALTERING SUBSTRATE SPECIFICITY OF CYTOCHROME C PEROXIDASE TOWARDS A SMALL MOLECULAR SUBSTRATE PEROXIDASE BY SUBSTITUTING TYROSINE FOR PHE 202
Authors : Cao, Y.; Musah, R.A.; Wilcox, S.K.; Goodin, D.B.; Mcree, D.E.
Deposited on : 1998-01-02
Resolution : 2.10 Å(reported)

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

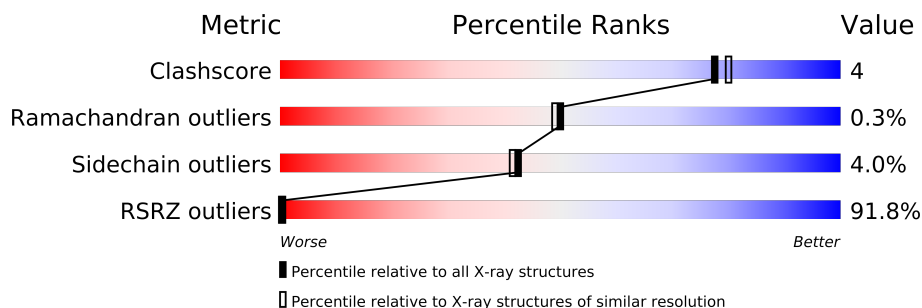
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	291	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3014 atoms, of which 513 are hydrogens and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

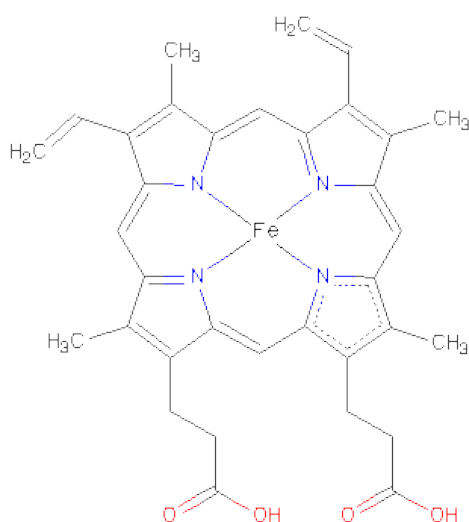
- Molecule 1 is a protein called CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	291	2864	1501	513	392	452	6	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	SUBSTITUTION	UNP P00431
A	152	GLY	ASP	SUBSTITUTION	UNP P00431
A	202	TYR	PHE	SUBSTITUTION	UNP P00431

- 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
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0

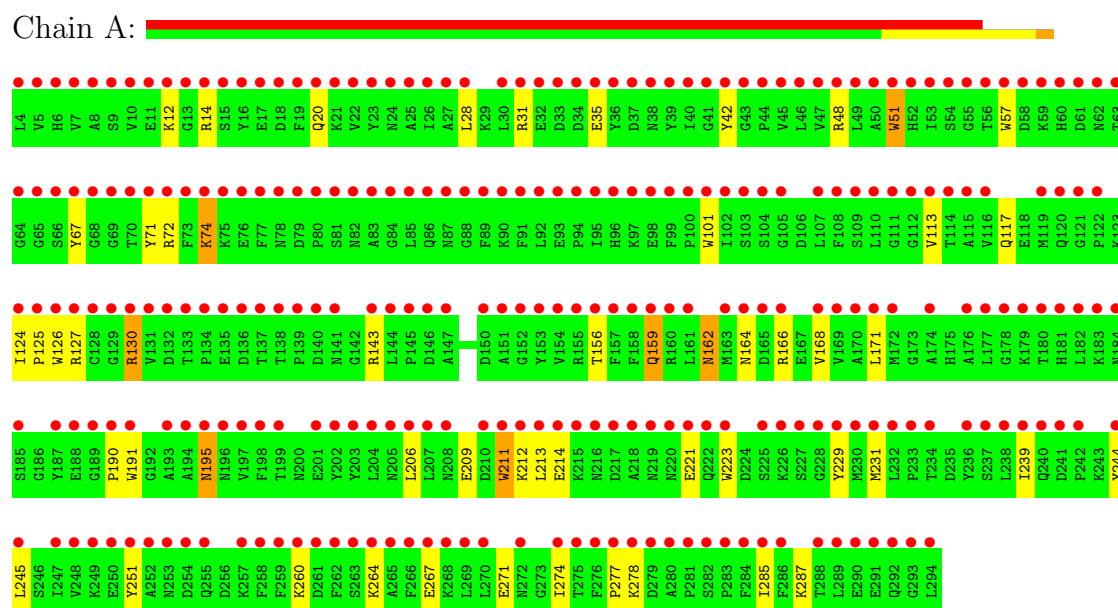
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total 107	O 107	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CYTOCHROME C PEROXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.50Å 73.40Å 44.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.10 18.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.10) 75.5 (18.77-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.90Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.184 , (Not available) 0.482 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 20709 reflections	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	3014	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

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	0.84	0/2417	1.56	39/3272 (1.2%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	A	127	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	31	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	A	143	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	A	51	TRP	CD1-CG-CD2	8.70	113.26	106.30
1	A	127	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	A	229	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	A	51	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	101	TRP	CD1-CG-CD2	7.81	112.55	106.30
1	A	211	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A	223	TRP	CD1-CG-CD2	7.60	112.38	106.30
1	A	191	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	A	211	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	A	126	TRP	CD1-CG-CD2	7.33	112.17	106.30
1	A	223	TRP	CE2-CD2-CG	-7.27	101.49	107.30
1	A	48	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	101	TRP	CE2-CD2-CG	-7.08	101.64	107.30
1	A	191	TRP	CD1-CG-CD2	6.81	111.75	106.30
1	A	57	TRP	CE2-CD2-CG	-6.73	101.92	107.30
1	A	72	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	51	TRP	CB-CG-CD1	-6.39	118.70	127.00
1	A	251	TYR	CB-CG-CD2	-6.34	117.20	121.00
1	A	57	TRP	CD1-CG-CD2	6.19	111.25	106.30
1	A	162	ASN	CA-C-N	-6.17	103.62	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	LYS	CA-CB-CG	-6.17	99.83	113.40
1	A	126	TRP	CE2-CD2-CG	-6.07	102.44	107.30
1	A	51	TRP	CG-CD1-NE1	-6.02	104.08	110.10
1	A	244	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	191	TRP	CG-CD2-CE3	5.85	139.16	133.90
1	A	72	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	101	TRP	CG-CD1-NE1	-5.49	104.61	110.10
1	A	42	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	31	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	191	TRP	CB-CG-CD1	-5.39	119.99	127.00
1	A	277	PRO	CA-C-N	5.36	129.00	117.20
1	A	51	TRP	CG-CD2-CE3	5.31	138.68	133.90
1	A	71	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	130	ARG	CG-CD-NE	-5.14	101.01	111.80
1	A	244	TYR	CB-CG-CD1	5.09	124.06	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2351	513	1716	17	22
2	A	43	0	30	0	0
3	A	107	0	0	3	8
All	All	2501	513	1746	17	22

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (17) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:206:LEU:HD13	1:A:231:MET:SD	2.45	0.56
1:A:113:VAL:HG13	1:A:124:ILE:HB	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:74:LYS:H	1:A:74:LYS:HD2	1.75	0.51
1:A:130:ARG:NE	3:A:326:HOH:O	2.44	0.51
1:A:164:ASN:O	1:A:168:VAL:HG23	2.13	0.47
1:A:67:TYR:O	1:A:130:ARG:HB3	2.15	0.46
1:A:156:THR:O	1:A:159:GLN:HB3	2.16	0.46
1:A:209:GLU:HB2	1:A:211:TRP:CE2	2.51	0.46
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.98	0.45
1:A:113:VAL:O	1:A:117:GLN:HG3	2.18	0.43
1:A:130:ARG:CZ	3:A:326:HOH:O	2.67	0.42
1:A:271:GLU:HA	1:A:274:ILE:HD12	2.01	0.42
1:A:195:ASN:HD22	1:A:195:ASN:H	1.67	0.42
1:A:239:ILE:HG22	1:A:245:LEU:HD13	2.01	0.41
1:A:20:GLN:NE2	1:A:287:LYS:H	2.19	0.41
1:A:213:LEU:HD11	1:A:221:GLU:HB3	2.03	0.41
1:A:267:GLU:HG3	3:A:323:HOH:O	2.22	0.40

All (22) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:ARG:NH2	1:A:213:LEU:C[4_5610]	0.92	1.28
1:A:212:LYS:CG	3:A:372:HOH:O[4_4610]	1.11	1.09
1:A:212:LYS:CE	3:A:374:HOH:O[4_4610]	1.34	0.86
1:A:212:LYS:CD	3:A:372:HOH:O[4_4610]	1.35	0.85
1:A:212:LYS:NZ	3:A:374:HOH:O[4_4610]	1.37	0.83
1:A:12:LYS:N	1:A:214:GLU:OE2[4_5610]	1.41	0.79
1:A:214:GLU:CG	3:A:373:HOH:O[4_4610]	1.48	0.72
1:A:12:LYS:O	1:A:214:GLU:CB[4_5610]	1.49	0.71
1:A:12:LYS:CB	1:A:214:GLU:OE2[4_5610]	1.50	0.70
1:A:14:ARG:NH2	1:A:214:GLU:N[4_5610]	1.52	0.68
1:A:14:ARG:NH2	1:A:213:LEU:O[4_5610]	1.53	0.67
1:A:264:LYS:NZ	3:A:389:HOH:O[3_559]	1.54	0.66
1:A:12:LYS:CA	1:A:214:GLU:OE2[4_5610]	1.55	0.65
1:A:212:LYS:CE	3:A:372:HOH:O[4_4610]	1.62	0.58
1:A:14:ARG:NE	1:A:213:LEU:O[4_5610]	1.71	0.49
1:A:12:LYS:CB	1:A:214:GLU:CD[4_5610]	1.77	0.43
1:A:14:ARG:CZ	1:A:213:LEU:O[4_5610]	1.78	0.42
1:A:12:LYS:CB	1:A:214:GLU:OE1[4_5610]	1.86	0.34
1:A:14:ARG:NH2	1:A:213:LEU:CA[4_5610]	1.87	0.33
1:A:14:ARG:CZ	1:A:213:LEU:C[4_5610]	2.01	0.19
1:A:212:LYS:CB	3:A:372:HOH:O[4_4610]	2.12	0.08
1:A:12:LYS:O	1:A:214:GLU:CG[4_5610]	2.19	0.01

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	289/291 (99%)	279 (96%)	9 (3%)	1 (0%)	50	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	ASN

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	249/249 (100%)	239 (96%)	10 (4%)	42	41

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	LEU
1	A	35	GLU
1	A	51	TRP
1	A	74	LYS
1	A	159	GLN
1	A	166	ARG
1	A	171	LEU
1	A	190	PRO
1	A	195	ASN
1	A	260	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	87	ASN
1	A	195	ASN
1	A	220	ASN
1	A	240	GLN
1	A	255	GLN
1	A	292	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	A	1	1,3	49,50,50	5.79	22 (44%)	46,82,82	1.39	4 (8%)

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	1	1,3	-	0/14/114/114	0/0/8/8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	HEM	C2D-C1D	-24.54	1.38	1.44
2	A	1	HEM	C3D-C4D	-23.20	1.38	1.44
2	A	1	HEM	C2B-C1B	-17.83	1.40	1.44
2	A	1	HEM	C3B-C4B	-3.69	1.40	1.44
2	A	1	HEM	C4C-NC	-3.66	1.32	1.38
2	A	1	HEM	FE-NB	3.16	2.09	1.97
2	A	1	HEM	C4D-ND	-3.11	1.33	1.39
2	A	1	HEM	CHB-C1B	3.10	1.40	1.35
2	A	1	HEM	CHA-C4D	3.09	1.40	1.35
2	A	1	HEM	C1B-NB	-3.06	1.33	1.39
2	A	1	HEM	C1A-C2A	-2.96	1.38	1.43
2	A	1	HEM	CBB-CAB	2.78	1.45	1.28
2	A	1	HEM	FE-ND	2.74	2.07	1.97
2	A	1	HEM	CBC-CAC	2.49	1.43	1.28
2	A	1	HEM	CHC-C1C	2.46	1.40	1.36
2	A	1	HEM	FE-NA	2.41	2.02	1.92
2	A	1	HEM	CHD-C4C	2.40	1.40	1.36
2	A	1	HEM	CMC-C2C	2.37	1.54	1.47
2	A	1	HEM	FE-NC	2.26	2.06	1.97
2	A	1	HEM	C3D-C2D	-2.22	1.39	1.43
2	A	1	HEM	CMB-C2B	2.20	1.54	1.47
2	A	1	HEM	C4A-C3A	-2.05	1.37	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	HEM	C3B-C4B-NB	-4.75	110.60	114.00
2	A	1	HEM	CMB-C2B-C3B	2.63	132.36	126.16
2	A	1	HEM	CHC-C1C-NC	-2.49	122.57	124.73
2	A	1	HEM	C4A-C3A-C2A	-2.19	105.47	107.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	291/291 (100%)	4.21	267 (91%) 0 0	10, 21, 36, 46	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	TRP	13.6
1	A	218	ALA	12.5
1	A	171	LEU	11.4
1	A	10	VAL	11.4
1	A	4	LEU	9.6
1	A	16	TYR	9.4
1	A	71	TYR	8.9
1	A	294	LEU	8.8
1	A	22	VAL	8.7
1	A	211	TRP	8.3
1	A	36	TYR	8.2
1	A	145	PRO	8.1
1	A	138	THR	7.8
1	A	53	ILE	7.7
1	A	286	PHE	7.7
1	A	67	TYR	7.5
1	A	12	LYS	7.3
1	A	251	TYR	7.2
1	A	124	ILE	7.1
1	A	83	ALA	7.1
1	A	206	LEU	7.1
1	A	187	TYR	7.1
1	A	275	THR	7.1
1	A	89	PHE	7.1
1	A	64	GLY	7.0
1	A	270	LEU	6.8
1	A	156	THR	6.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	169	VAL	6.8
1	A	46	LEU	6.8
1	A	153	TYR	6.8
1	A	203	TYR	6.8
1	A	5	VAL	6.7
1	A	282	SER	6.6
1	A	231	MET	6.6
1	A	219	ASN	6.4
1	A	276	PHE	6.4
1	A	247	ILE	6.3
1	A	277	PRO	6.2
1	A	161	LEU	6.2
1	A	38	ASN	6.1
1	A	65	GLY	6.1
1	A	63	THR	6.1
1	A	269	LEU	6.1
1	A	28	LEU	6.0
1	A	213	LEU	6.0
1	A	202	TYR	5.9
1	A	230	MET	5.8
1	A	30	LEU	5.8
1	A	109	SER	5.7
1	A	41	GLY	5.7
1	A	61	ASP	5.7
1	A	278	LYS	5.7
1	A	259	PHE	5.6
1	A	177	LEU	5.6
1	A	49	LEU	5.6
1	A	288	THR	5.6
1	A	25	ALA	5.5
1	A	40	ILE	5.5
1	A	77	PHE	5.5
1	A	42	TYR	5.5
1	A	283	PRO	5.5
1	A	191	TRP	5.5
1	A	23	TYR	5.4
1	A	244	TYR	5.4
1	A	128	CYS	5.4
1	A	79	ASP	5.3
1	A	8	ALA	5.3
1	A	7	VAL	5.3
1	A	198	PHE	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	85	LEU	5.3
1	A	236	TYR	5.3
1	A	108	PHE	5.2
1	A	6	HIS	5.2
1	A	62	ASN	5.1
1	A	141	ASN	5.1
1	A	228	GLY	5.1
1	A	19	PHE	5.1
1	A	133	THR	5.1
1	A	234	THR	5.1
1	A	39	TYR	5.1
1	A	57	TRP	5.0
1	A	131	VAL	5.0
1	A	9	SER	5.0
1	A	217	ASP	5.0
1	A	52	HIS	5.0
1	A	159	GLN	5.0
1	A	97	LYS	5.0
1	A	105	GLY	5.0
1	A	193	ALA	4.9
1	A	126	TRP	4.9
1	A	66	SER	4.9
1	A	144	LEU	4.9
1	A	207	LEU	4.8
1	A	252	ALA	4.8
1	A	291	GLU	4.7
1	A	266	PHE	4.7
1	A	33	ASP	4.7
1	A	75	LYS	4.7
1	A	73	PHE	4.7
1	A	274	ILE	4.7
1	A	45	VAL	4.6
1	A	262	PHE	4.6
1	A	284	PHE	4.6
1	A	229	TYR	4.6
1	A	35	GLU	4.6
1	A	13	GLY	4.5
1	A	26	ILE	4.5
1	A	254	ASP	4.5
1	A	292	GLN	4.5
1	A	240	GLN	4.4
1	A	293	GLY	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	44	PRO	4.4
1	A	205	ASN	4.4
1	A	11	GLU	4.3
1	A	248	VAL	4.3
1	A	37	ASP	4.3
1	A	92	LEU	4.3
1	A	258	PHE	4.3
1	A	279	ASP	4.3
1	A	15	SER	4.2
1	A	170	ALA	4.2
1	A	245	LEU	4.2
1	A	197	VAL	4.2
1	A	127	ARG	4.2
1	A	14	ARG	4.2
1	A	101	TRP	4.2
1	A	70	THR	4.2
1	A	125	PRO	4.2
1	A	263	SER	4.2
1	A	154	VAL	4.1
1	A	51	TRP	4.1
1	A	255	GLN	4.1
1	A	34	ASP	4.1
1	A	249	LYS	4.1
1	A	107	LEU	4.0
1	A	87	ASN	4.0
1	A	139	PRO	4.0
1	A	147	ALA	4.0
1	A	116	VAL	4.0
1	A	215	LYS	4.0
1	A	115	ALA	3.9
1	A	226	LYS	3.9
1	A	60	HIS	3.9
1	A	158	PHE	3.9
1	A	104	SER	3.9
1	A	265	ALA	3.9
1	A	190	PRO	3.9
1	A	214	GLU	3.8
1	A	114	THR	3.8
1	A	216	ASN	3.8
1	A	110	LEU	3.8
1	A	122	PRO	3.8
1	A	250	GLU	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	3.8
1	A	268	LYS	3.8
1	A	27	ALA	3.8
1	A	189	GLY	3.8
1	A	91	PHE	3.7
1	A	102	ILE	3.7
1	A	242	PRO	3.7
1	A	157	PHE	3.7
1	A	168	VAL	3.7
1	A	264	LYS	3.7
1	A	78	ASN	3.7
1	A	238	LEU	3.6
1	A	196	ASN	3.6
1	A	166	ARG	3.6
1	A	233	PRO	3.6
1	A	48	ARG	3.6
1	A	55	GLY	3.6
1	A	182	LEU	3.6
1	A	20	GLN	3.5
1	A	76	GLU	3.5
1	A	72	ARG	3.5
1	A	136	ASP	3.5
1	A	237	SER	3.5
1	A	74	LYS	3.5
1	A	113	VAL	3.5
1	A	220	ASN	3.5
1	A	241	ASP	3.4
1	A	132	ASP	3.4
1	A	31	ARG	3.4
1	A	21	LYS	3.3
1	A	225	SER	3.3
1	A	204	LEU	3.3
1	A	165	ASP	3.3
1	A	47	VAL	3.3
1	A	32	GLU	3.3
1	A	222	GLN	3.3
1	A	137	THR	3.3
1	A	199	THR	3.2
1	A	180	THR	3.2
1	A	95	ILE	3.2
1	A	80	PRO	3.2
1	A	239	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	93	GLU	3.2
1	A	81	SER	3.2
1	A	290	GLU	3.1
1	A	56	THR	3.1
1	A	155	ARG	3.1
1	A	59	LYS	3.1
1	A	289	LEU	3.1
1	A	201	GLU	3.1
1	A	135	GLU	3.1
1	A	99	PHE	3.0
1	A	188	GLU	3.0
1	A	281	PRO	3.0
1	A	164	ASN	3.0
1	A	183	LYS	2.9
1	A	17	GLU	2.9
1	A	50	ALA	2.9
1	A	103	SER	2.9
1	A	143	ARG	2.8
1	A	253	ASN	2.8
1	A	232	LEU	2.8
1	A	227	SER	2.8
1	A	221	GLU	2.8
1	A	54	SER	2.8
1	A	174	ALA	2.8
1	A	68	GLY	2.8
1	A	163	MET	2.8
1	A	195	ASN	2.7
1	A	179	LYS	2.7
1	A	160	ARG	2.7
1	A	134	PRO	2.7
1	A	121	GLY	2.7
1	A	210	ASP	2.7
1	A	194	ALA	2.7
1	A	172	MET	2.7
1	A	185	SER	2.7
1	A	43	GLY	2.7
1	A	82	ASN	2.6
1	A	69	GLY	2.6
1	A	130	ARG	2.6
1	A	184	ASN	2.6
1	A	100	PRO	2.6
1	A	90	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	285	ILE	2.6
1	A	261	ASP	2.6
1	A	129	GLY	2.5
1	A	181	HIS	2.5
1	A	257	LYS	2.5
1	A	24	ASN	2.5
1	A	272	ASN	2.5
1	A	119	MET	2.5
1	A	146	ASP	2.5
1	A	96	HIS	2.4
1	A	152	GLY	2.4
1	A	212	LYS	2.4
1	A	94	PRO	2.4
1	A	176	ALA	2.3
1	A	18	ASP	2.3
1	A	98	GLU	2.3
1	A	280	ALA	2.3
1	A	120	GLN	2.2
1	A	267	GLU	2.2
1	A	208	ASN	2.2
1	A	111	GLY	2.2
1	A	84	GLY	2.2
1	A	178	GLY	2.1
1	A	86	GLN	2.1
1	A	88	GLY	2.1
1	A	260	LYS	2.1
1	A	151	ALA	2.1
1	A	58	ASP	2.0
1	A	112	GLY	2.0
1	A	150	ASP	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEM	A	1	43/43	0.33	-0.43	9,14,18,24	0

6.5 Other polymers

There are no such residues in this entry.