



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 12, 2019 – 08:01 PM EST

PDB ID : 4AX3  
Title : Structure of three-domain heme-Cu nitrite reductase from *Ralstonia pickettii* at 1.6 Å resolution  
Authors : Antonyuk, S.V.; Cong, H.; Eady, R.R.; Hasnain, S.S.  
Deposited on : 2012-06-07  
Resolution : 1.60 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031633
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)	:	rb-20031633

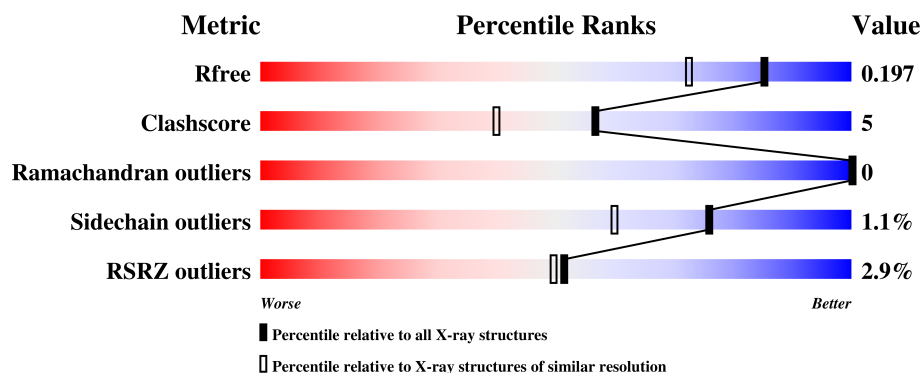
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2957 (1.60-1.60)
Clashscore	122126	3202 (1.60-1.60)
Ramachandran outliers	120053	3117 (1.60-1.60)
Sidechain outliers	120020	3116 (1.60-1.60)
RSRZ outliers	108989	2883 (1.60-1.60)

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	468	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	B	468	<div> <div>%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	C	468	<div> <div>%</div> <div>88%</div> <div>9%</div> <div>.</div> </div>
1	D	468	<div> <div>7%</div> <div>89%</div> <div>9%</div> <div>.</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16795 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.

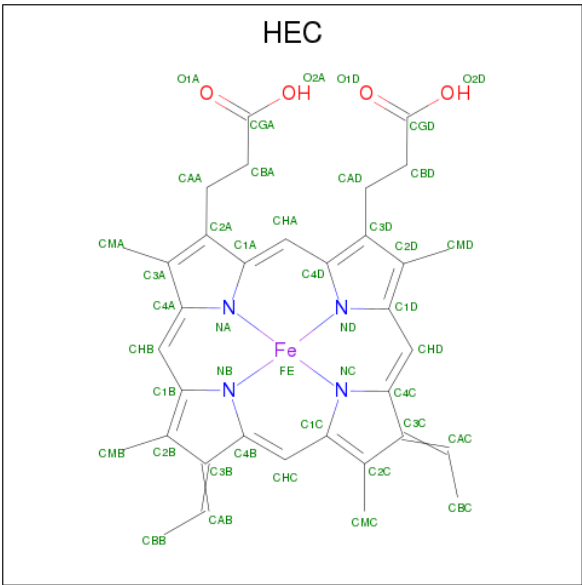
- Molecule 1 is a protein called COPPER-CONTAINING NITRITE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	456	Total	C	N	O	S	0	21	0
			3551	2270	610	655	16			
1	B	455	Total	C	N	O	S	0	21	0
			3543	2260	607	661	15			
1	C	455	Total	C	N	O	S	0	22	0
			3547	2264	603	664	16			
1	D	457	Total	C	N	O	S	0	9	0
			3495	2225	603	652	15			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	0
			2	2		
2	A	2	Total	Cu	0	0
			2	2		
2	D	2	Total	Cu	0	0
			2	2		
2	C	2	Total	Cu	0	0
			2	2		

- Molecule 3 is HEME C (three-letter code: HEC) (formula: C<sub>34</sub>H<sub>34</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

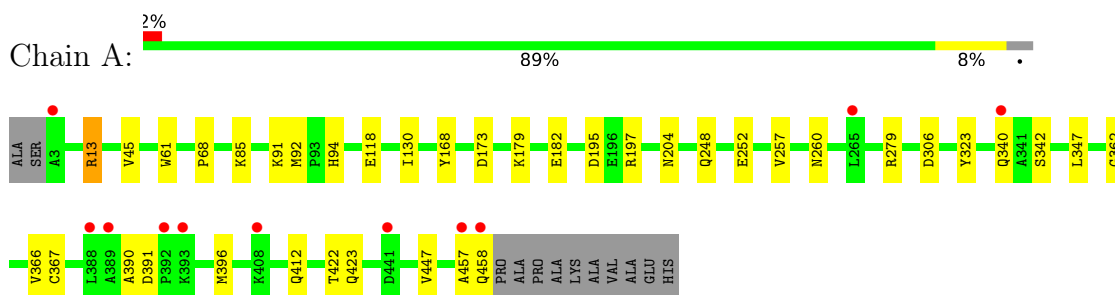
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	629	Total	O	0	7
			636	636		
4	B	633	Total	O	0	2
			635	635		
4	C	697	Total	O	0	0
			697	697		
4	D	511	Total	O	0	0
			511	511		

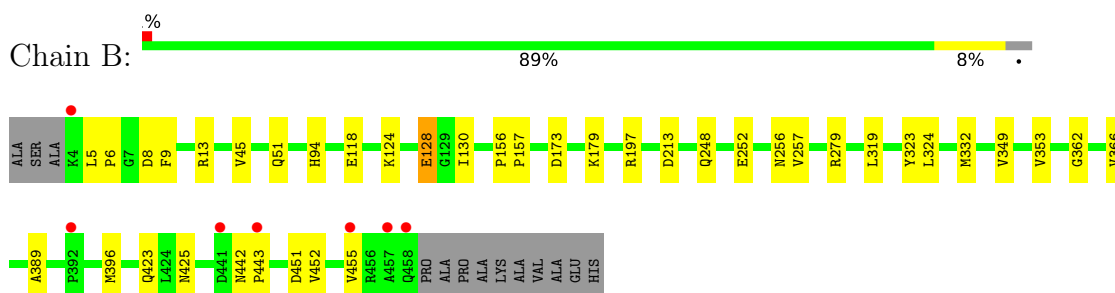
### 3 Residue-property plots [i](#)

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.

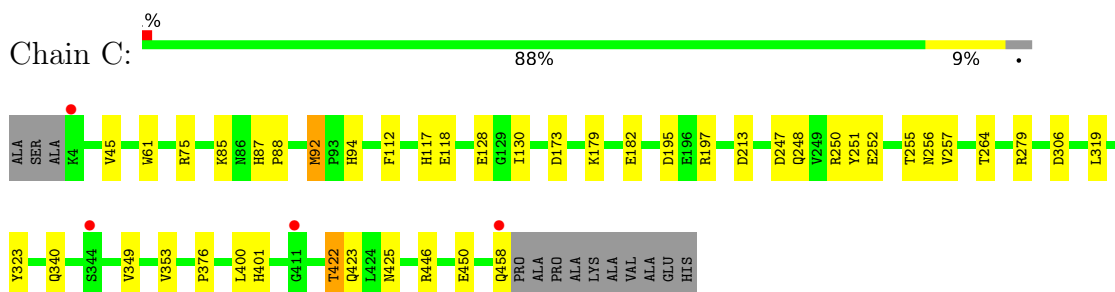
#### • Molecule 1: COPPER-CONTAINING NITRITE REDUCTASE



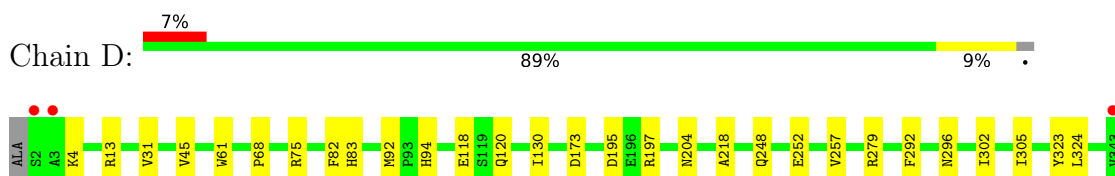
#### • Molecule 1: COPPER-CONTAINING NITRITE REDUCTASE

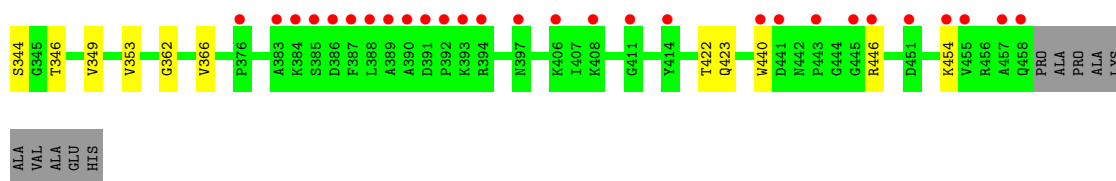


#### • Molecule 1: COPPER-CONTAINING NITRITE REDUCTASE



#### • Molecule 1: COPPER-CONTAINING NITRITE REDUCTASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.81Å 185.81Å 185.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.60 49.66 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (25.00-1.60) 99.8 (49.66-1.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.163 , 0.194 0.168 , 0.197	Depositor DCC
$R_{free}$ test set	14067 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16795	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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 46.17 % 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 1.1891e-04. 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CU, HEC

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	0.70	0/3700	0.75	1/5026 (0.0%)
1	B	0.74	4/3687 (0.1%)	0.77	2/5009 (0.0%)
1	C	0.78	0/3698	0.82	5/5022 (0.1%)
1	D	0.68	0/3607	0.71	0/4898
All	All	0.73	4/14692 (0.0%)	0.76	8/19955 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128[A]	GLU	CB-CG	-7.04	1.38	1.52
1	B	128[B]	GLU	CB-CG	-7.04	1.38	1.52
1	B	128[A]	GLU	CD-OE2	-5.71	1.19	1.25
1	B	128[B]	GLU	CD-OE2	-5.71	1.19	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	MET	CG-SD-CE	-6.38	90.00	100.20
1	C	446	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	75	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	247	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	C	279	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	168	TYR	CB-CG-CD1	5.25	124.15	121.00
1	C	319	LEU	CA-CB-CG	5.24	127.35	115.30
1	B	279	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3551	0	3578	45	0
1	B	3543	0	3544	37	0
1	C	3547	0	3556	39	0
1	D	3495	0	3477	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	43	0	30	3	0
3	B	43	0	30	2	0
3	C	43	0	30	1	0
3	D	43	0	30	2	0
4	A	636	0	0	25	0
4	B	635	0	0	12	0
4	C	697	0	0	19	1
4	D	511	0	0	8	0
All	All	16795	0	14275	152	1

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 5.

All (152) 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:13[A]:ARG:NH2	4:A:2036:HOH:O	1.57	1.35
1:B:51[B]:GLN:NE2	4:B:2130:HOH:O	1.60	1.25
1:A:412[A]:GLN:NE2	4:A:2599:HOH:O	1.64	1.24
1:A:260[B]:ASN:ND2	4:A:2462:HOH:O	1.71	1.23
1:B:118:GLU:OE2	4:B:2206:HOH:O	1.52	1.21
1:D:423[B]:GLN:OE1	4:D:2488:HOH:O	1.63	1.16
1:B:423[B]:GLN:OE1	4:B:2596:HOH:O	1.61	1.14
1:C:306[A]:ASP:OD1	4:C:2506:HOH:O	1.67	1.12
1:B:396:MET:HE2	1:B:455:VAL:HG21	1.29	1.12
1:A:179[B]:LYS:HE2	4:A:2351:HOH:O	0.94	1.11
1:A:306[A]:ASP:OD1	4:A:2492:HOH:O	1.67	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423[B]:GLN:OE1	4:C:2652:HOH:O	1.67	1.10
1:A:260[B]:ASN:OD1	4:A:2431:HOH:O	1.69	1.08
1:B:197[B]:ARG:HD2	4:B:2371:HOH:O	1.58	1.02
1:A:306[B]:ASP:OD2	4:A:2496:HOH:O	1.80	1.00
1:A:306[A]:ASP:CG	4:A:2492:HOH:O	2.00	0.96
1:B:213[B]:ASP:OD1	4:B:2387:HOH:O	1.82	0.96
1:B:213[B]:ASP:OD2	4:B:2390:HOH:O	1.84	0.95
1:B:396:MET:HE2	1:B:455:VAL:CG2	1.97	0.95
1:C:182[A]:GLU:OE1	4:C:2703:HOH:O	1.87	0.93
1:A:91[A]:LYS:HE3	4:A:2240:HOH:O	1.69	0.90
1:B:362:GLY:O	1:B:366[B]:VAL:HG13	1.74	0.88
1:C:213[B]:ASP:OD1	4:C:2421:HOH:O	1.90	0.88
1:A:306[A]:ASP:OD2	4:A:2492:HOH:O	1.91	0.88
1:C:264[B]:THR:HG23	1:C:264[B]:THR:O	1.73	0.88
1:D:279[A]:ARG:CZ	4:D:2362:HOH:O	2.23	0.86
1:C:85[B]:LYS:HE2	1:C:118[B]:GLU:OE2	1.75	0.86
1:A:279[B]:ARG:HD3	4:A:2645:HOH:O	1.76	0.85
1:C:195[B]:ASP:OD2	1:C:197[B]:ARG:HD2	1.76	0.84
1:A:248[A]:GLN:NE2	4:A:2436:HOH:O	2.12	0.81
1:B:396:MET:HE3	1:B:452:VAL:HA	1.61	0.80
1:B:396:MET:CE	1:B:455:VAL:CG2	2.60	0.79
1:A:423[A]:GLN:NE2	4:A:2611:HOH:O	2.12	0.76
1:C:306[A]:ASP:CG	4:C:2506:HOH:O	2.16	0.75
1:C:400:LEU:O	1:C:422[B]:THR:HG22	1.85	0.74
1:C:197[A]:ARG:HD3	4:C:2392:HOH:O	1.85	0.74
1:B:396:MET:CE	1:B:455:VAL:HG21	2.15	0.73
1:B:396:MET:HE1	1:B:451:ASP:O	1.88	0.72
1:A:91[A]:LYS:CE	4:A:2240:HOH:O	2.27	0.71
1:C:248[A]:GLN:NE2	4:C:2453:HOH:O	2.02	0.69
1:A:85[B]:LYS:HG3	4:A:2073:HOH:O	1.90	0.68
1:D:83:HIS:ND1	4:D:2157:HOH:O	2.25	0.68
1:A:13[B]:ARG:NH1	4:A:2035:HOH:O	2.26	0.68
1:A:367:CYS:SG	3:A:600:HEC:CBC	2.79	0.68
1:A:248[B]:GLN:HG3	1:A:257:VAL:CG1	2.23	0.67
1:A:279[B]:ARG:CZ	4:A:2477:HOH:O	2.43	0.67
1:B:248:GLN:HG3	1:B:257:VAL:CG1	2.24	0.67
1:A:91[A]:LYS:NZ	4:A:2240:HOH:O	2.27	0.66
1:C:306[A]:ASP:OD2	4:C:2506:HOH:O	2.13	0.66
1:C:340[B]:GLN:OE1	4:C:2559:HOH:O	2.15	0.65
1:A:179[B]:LYS:CE	4:A:2351:HOH:O	1.77	0.64
1:A:367:CYS:SG	3:A:600:HEC:C3C	2.84	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248[B]:GLN:CG	1:D:257:VAL:CG1	2.76	0.64
1:C:85[B]:LYS:HE2	1:C:118[B]:GLU:CD	2.18	0.63
1:A:340[A]:GLN:HG3	4:A:2544:HOH:O	2.00	0.62
1:B:396:MET:CE	1:B:452:VAL:HA	2.28	0.62
3:C:600:HEC:HMC1	3:C:600:HEC:HBC3	1.82	0.62
1:A:85[B]:LYS:HE2	1:A:118:GLU:OE2	2.01	0.61
1:D:4:LYS:NZ	4:D:2003:HOH:O	0.76	0.60
1:C:179:LYS:HE2	1:C:425:ASN:ND2	2.16	0.60
1:C:255:THR:HG21	4:C:2468:HOH:O	2.01	0.60
1:C:85[B]:LYS:CE	1:C:118[B]:GLU:OE2	2.49	0.60
1:D:248[B]:GLN:HG3	1:D:257:VAL:CG1	2.33	0.59
1:A:182[A]:GLU:OE1	4:A:2347:HOH:O	2.16	0.59
1:B:118:GLU:HG2	4:B:2206:HOH:O	2.03	0.58
1:D:195[B]:ASP:OD2	1:D:197:ARG:HD2	2.03	0.58
1:A:279[B]:ARG:NH1	4:A:2477:HOH:O	2.36	0.58
1:B:197[A]:ARG:HD3	4:B:2371:HOH:O	2.03	0.58
1:C:45:VAL:HG11	1:C:94:HIS:CD2	2.39	0.57
3:B:600:HEC:HBB3	3:B:600:HEC:HMB1	1.86	0.57
1:D:349:VAL:HG23	1:D:446:ARG:HH21	1.69	0.57
3:D:600:HEC:HMB1	3:D:600:HEC:HBB3	1.86	0.57
1:A:396:MET:HE1	1:A:447:VAL:HG13	1.86	0.56
1:B:9:PHE:CE2	1:B:157[B]:PRO:HG3	2.41	0.56
1:A:396:MET:CE	1:A:447:VAL:HG13	2.37	0.54
1:A:457:ALA:O	1:A:458:GLN:HB2	2.07	0.54
1:B:118:GLU:CG	4:B:2206:HOH:O	2.56	0.54
1:C:340[B]:GLN:NE2	4:C:2565:HOH:O	2.41	0.53
1:D:349:VAL:O	1:D:353:VAL:HG23	2.09	0.53
1:B:256:ASN:ND2	4:B:2434:HOH:O	2.37	0.52
1:C:130:ILE:O	1:C:252:GLU:HA	2.09	0.52
1:C:450[B]:GLU:HG3	4:C:2351:HOH:O	2.09	0.52
1:D:45:VAL:HG11	1:D:94:HIS:CD2	2.45	0.52
1:C:197[A]:ARG:CG	4:C:2392:HOH:O	2.58	0.52
1:A:85[B]:LYS:CG	4:A:2073:HOH:O	2.56	0.51
1:D:366:VAL:HG11	4:D:2447:HOH:O	2.10	0.51
1:D:197:ARG:HD3	4:D:2284:HOH:O	2.10	0.51
3:A:600:HEC:HBB3	3:A:600:HEC:HMB1	1.92	0.50
1:A:362:GLY:O	1:A:366[B]:VAL:HG23	2.11	0.50
1:B:442:ASN:HB3	1:B:443:PRO:HD2	1.92	0.50
1:D:446:ARG:HD2	4:D:2504:HOH:O	2.11	0.50
1:C:195[B]:ASP:HB3	1:C:197[B]:ARG:HG3	1.92	0.50
3:B:600:HEC:HMC1	3:B:600:HEC:HBC3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ASN:ND2	4:C:2469:HOH:O	2.43	0.49
1:B:389:ALA:HB3	1:C:376:PRO:HG2	1.95	0.49
1:B:179[B]:LYS:HE2	1:B:425:ASN:OD1	2.12	0.49
1:B:362:GLY:O	1:B:366[A]:VAL:HG12	2.13	0.48
3:D:600:HEC:HMC1	3:D:600:HEC:HBC3	1.97	0.47
1:C:61:TRP:CH2	1:C:92[B]:MET:HG3	2.49	0.47
1:A:130:ILE:O	1:A:252:GLU:HA	2.15	0.47
1:A:13[A]:ARG:CZ	4:A:2036:HOH:O	2.27	0.47
1:A:248[B]:GLN:HG3	1:A:257:VAL:HG13	1.97	0.47
1:B:130:ILE:O	1:B:252:GLU:HA	2.15	0.46
1:D:130:ILE:O	1:D:252:GLU:HA	2.15	0.46
1:B:128[A]:GLU:HG3	1:B:156:PRO:HA	1.97	0.46
1:C:128[A]:GLU:OE2	1:C:250:ARG:NH1	2.42	0.46
1:C:248[B]:GLN:HG3	1:C:257:VAL:CG1	2.46	0.46
1:C:401:HIS:HE1	4:C:2629:HOH:O	2.00	0.45
1:B:8[B]:ASP:CG	1:B:124[B]:LYS:HZ3	2.20	0.45
1:A:68:PRO:HD3	1:A:204:ASN:HA	1.99	0.44
1:B:128[A]:GLU:HG3	1:B:156:PRO:CA	2.48	0.44
1:C:112:PHE:HB2	4:C:2239:HOH:O	2.18	0.44
1:A:13[A]:ARG:CD	4:A:2037:HOH:O	2.62	0.44
1:C:195[B]:ASP:OD2	1:C:197[B]:ARG:CD	2.59	0.43
1:A:248[B]:GLN:CG	1:A:257:VAL:CG1	2.95	0.43
1:A:390:ALA:O	1:D:440:TRP:HA	2.18	0.43
1:D:248[B]:GLN:CD	1:D:257:VAL:HG11	2.38	0.43
1:B:396:MET:HE1	1:B:455:VAL:HG23	1.98	0.43
1:A:45:VAL:HG11	1:A:94:HIS:CD2	2.53	0.43
1:B:349:VAL:O	1:B:353:VAL:HG23	2.19	0.43
1:D:118:GLU:HG2	4:D:2157:HOH:O	2.17	0.43
1:D:344:SER:HB2	1:D:346:THR:HG22	2.01	0.43
1:D:82:PHE:O	1:D:120:GLN:HA	2.19	0.43
1:A:61:TRP:CH2	1:A:92[A]:MET:HG3	2.54	0.42
1:C:85[B]:LYS:HG2	1:C:118[B]:GLU:CG	2.48	0.42
1:D:61:TRP:CH2	1:D:92:MET:HG3	2.53	0.42
1:A:248[B]:GLN:CG	1:A:257:VAL:HG13	2.48	0.42
1:D:292:PHE:O	1:D:296:ASN:HB2	2.18	0.42
1:D:68:PRO:HD3	1:D:204:ASN:HA	2.01	0.42
1:B:319:LEU:HD21	1:B:324:LEU:HD13	2.02	0.42
1:D:362:GLY:O	1:D:366:VAL:HG12	2.19	0.42
1:B:5:LEU:O	1:B:8[A]:ASP:HB2	2.20	0.41
1:D:302:ILE:HD11	1:D:324:LEU:HD21	2.01	0.41
1:C:85[B]:LYS:HG3	4:C:2126:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422[B]:THR:HG21	4:C:2654:HOH:O	2.20	0.41
1:C:349:VAL:O	1:C:353:VAL:HG23	2.20	0.41
1:A:195[A]:ASP:HB3	1:A:197[A]:ARG:HG3	2.02	0.41
1:A:390:ALA:O	1:A:391:ASP:HB2	2.21	0.41
1:A:342:SER:OG	1:A:347:LEU:HD22	2.21	0.41
1:B:197[B]:ARG:NH2	4:B:2370:HOH:O	2.45	0.41
1:B:45:VAL:HG11	1:B:94:HIS:CD2	2.56	0.41
1:D:31:VAL:HG21	1:D:75:ARG:HB2	2.03	0.41
1:A:457:ALA:O	1:A:458:GLN:CB	2.69	0.40
1:B:197[B]:ARG:HD2	4:B:2192:HOH:O	2.20	0.40
1:C:87:HIS:CG	1:C:88:PRO:HD2	2.57	0.40
1:B:5:LEU:HB3	1:B:6:PRO:HD2	2.04	0.40
1:C:458:GLN:C	4:C:2695:HOH:O	2.60	0.40
1:D:248[B]:GLN:CG	1:D:257:VAL:HG11	2.52	0.40
1:B:13[B]:ARG:HB2	1:B:13[B]:ARG:HE	1.72	0.40
1:D:218:ALA:HB3	1:D:305:ILE:CD1	2.51	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
4:C:2392:HOH:O	4:C:2392:HOH:O[6_456]	1.81	0.39

## 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	475/468 (102%)	465 (98%)	10 (2%)	0	100	100
1	B	474/468 (101%)	466 (98%)	8 (2%)	0	100	100
1	C	475/468 (102%)	468 (98%)	7 (2%)	0	100	100
1	D	464/468 (99%)	458 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1888/1872 (101%)	1857 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	384/371 (104%)	379 (99%)	5 (1%)	71	53
1	B	383/371 (103%)	381 (100%)	2 (0%)	90	82
1	C	385/371 (104%)	378 (98%)	7 (2%)	62	38
1	D	373/371 (100%)	367 (98%)	6 (2%)	65	44
All	All	1525/1484 (103%)	1505 (99%)	20 (1%)	76	53

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13[A]	ARG
1	A	13[B]	ARG
1	A	173	ASP
1	A	323	TYR
1	A	422	THR
1	B	173	ASP
1	B	323	TYR
1	C	92[A]	MET
1	C	92[B]	MET
1	C	117	HIS
1	C	173	ASP
1	C	323	TYR
1	C	422[A]	THR
1	C	422[B]	THR
1	D	13[A]	ARG
1	D	13[B]	ARG
1	D	173	ASP

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Mol	Chain	Res	Type
1	D	323	TYR
1	D	422	THR
1	D	454	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	397	ASN
1	C	260	ASN
1	C	425	ASN

### 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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z  > 2$
3	HEC	A	600	1	26,50,50	2.42	6 (23%)	18,82,82	2.10	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	HEC	B	600	1	26,50,50	2.61	9 (34%)	18,82,82	1.92	7 (38%)
3	HEC	C	600	1	26,50,50	2.40	8 (30%)	18,82,82	2.01	5 (27%)
3	HEC	D	600	1	26,50,50	2.40	7 (26%)	18,82,82	1.92	8 (44%)

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
3	HEC	A	600	1	-	0/6/54/54	0/0/8/8
3	HEC	B	600	1	-	0/6/54/54	0/0/8/8
3	HEC	C	600	1	-	0/6/54/54	0/0/8/8
3	HEC	D	600	1	-	0/6/54/54	0/0/8/8

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	HEC	C3C-C2C	-7.46	1.32	1.40
3	B	600	HEC	C3C-C2C	-6.92	1.33	1.40
3	A	600	HEC	C3B-C2B	-6.44	1.33	1.40
3	D	600	HEC	C3C-C2C	-6.43	1.33	1.40
3	B	600	HEC	C3B-C2B	-6.23	1.34	1.40
3	D	600	HEC	C3B-C2B	-5.73	1.34	1.40
3	A	600	HEC	C3C-C2C	-5.01	1.35	1.40
3	C	600	HEC	C3B-C2B	-4.26	1.36	1.40
3	A	600	HEC	CBC-CAC	-3.72	1.35	1.49
3	A	600	HEC	CBB-CAB	-3.54	1.35	1.49
3	B	600	HEC	CBB-CAB	-3.48	1.35	1.49
3	B	600	HEC	CBC-CAC	-3.44	1.36	1.49
3	D	600	HEC	CBB-CAB	-3.34	1.36	1.49
3	D	600	HEC	CBC-CAC	-3.33	1.36	1.49
3	C	600	HEC	CBB-CAB	-2.83	1.38	1.49
3	C	600	HEC	CBC-CAC	-2.60	1.39	1.49
3	B	600	HEC	C1D-ND	2.05	1.40	1.36
3	B	600	HEC	CMC-C2C	2.11	1.56	1.51
3	C	600	HEC	CMC-C2C	2.16	1.56	1.51
3	D	600	HEC	CAD-C3D	2.21	1.55	1.52
3	C	600	HEC	C1B-NB	2.25	1.40	1.36
3	A	600	HEC	C4D-ND	2.43	1.41	1.36
3	B	600	HEC	C4D-ND	2.48	1.41	1.36
3	D	600	HEC	C4D-ND	2.59	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	600	HEC	C4D-ND	2.91	1.42	1.36
3	B	600	HEC	CAD-C3D	2.95	1.57	1.52
3	C	600	HEC	C3D-C2D	4.31	1.50	1.37
3	D	600	HEC	C3D-C2D	4.57	1.51	1.37
3	B	600	HEC	C3D-C2D	4.58	1.51	1.37
3	A	600	HEC	C3D-C2D	4.76	1.51	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	600	HEC	C1D-C2D-C3D	-4.87	103.61	107.00
3	A	600	HEC	CMC-C2C-C1C	-4.28	121.89	128.46
3	A	600	HEC	C1D-C2D-C3D	-3.96	104.24	107.00
3	B	600	HEC	C1D-C2D-C3D	-3.21	104.76	107.00
3	B	600	HEC	C3C-C4C-NC	-3.07	105.15	110.94
3	D	600	HEC	CMC-C2C-C1C	-3.03	123.81	128.46
3	B	600	HEC	CMC-C2C-C1C	-2.80	124.16	128.46
3	A	600	HEC	CBD-CAD-C3D	-2.77	107.18	112.48
3	C	600	HEC	C3C-C4C-NC	-2.75	105.75	110.94
3	B	600	HEC	CBD-CAD-C3D	-2.66	107.41	112.48
3	D	600	HEC	CMB-C2B-C1B	-2.56	124.53	128.46
3	D	600	HEC	C1D-C2D-C3D	-2.43	105.30	107.00
3	A	600	HEC	C3C-C4C-NC	-2.43	106.36	110.94
3	D	600	HEC	C3B-C4B-NB	-2.34	106.53	110.94
3	B	600	HEC	CAD-C3D-C2D	-2.12	122.94	129.00
3	D	600	HEC	C3C-C4C-NC	-2.12	106.94	110.94
3	D	600	HEC	CBD-CAD-C3D	-2.05	108.56	112.48
3	C	600	HEC	CMB-C2B-C3B	2.22	128.43	125.82
3	A	600	HEC	CMA-C3A-C2A	2.35	129.37	124.94
3	C	600	HEC	CAA-CBA-CGA	2.53	116.98	112.66
3	B	600	HEC	C4C-C3C-C2C	2.57	109.13	106.35
3	B	600	HEC	CMA-C3A-C2A	2.60	129.85	124.94
3	D	600	HEC	CMB-C2B-C3B	2.73	129.03	125.82
3	D	600	HEC	C4B-C3B-C2B	3.10	109.70	106.35
3	A	600	HEC	CMC-C2C-C3C	3.10	129.47	125.82
3	C	600	HEC	C4B-C3B-C2B	3.29	109.91	106.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	HEC	3	0
3	B	600	HEC	2	0
3	C	600	HEC	1	0
3	D	600	HEC	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	456/468 (97%)	-0.04	11 (2%) 59 57	12, 20, 45, 58	11 (2%)
1	B	455/468 (97%)	-0.13	7 (1%) 73 74	12, 19, 38, 50	8 (1%)
1	C	455/468 (97%)	-0.27	4 (0%) 84 84	10, 18, 33, 44	5 (1%)
1	D	457/468 (97%)	0.02	31 (6%) 17 16	15, 24, 42, 49	13 (2%)
All	All	1823/1872 (97%)	-0.11	53 (2%) 51 49	10, 20, 41, 58	37 (2%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	389	ALA	6.0
1	A	389	ALA	4.9
1	A	3	ALA	4.7
1	D	387	PHE	4.5
1	B	4	LYS	4.4
1	B	457	ALA	4.4
1	D	392	PRO	4.2
1	A	457	ALA	4.1
1	D	390	ALA	4.1
1	D	411	GLY	3.7
1	D	2	SER	3.5
1	A	458	GLN	3.5
1	B	458	GLN	3.5
1	D	384	LYS	3.3
1	D	457	ALA	3.2
1	C	411	GLY	3.2
1	D	443	PRO	3.2
1	D	406	LYS	3.1
1	C	4	LYS	3.1
1	D	397	ASN	3.0
1	D	391	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	454	LYS	2.8
1	D	445	GLY	2.8
1	D	386	ASP	2.8
1	D	458	GLN	2.8
1	D	414	TYR	2.7
1	C	458	GLN	2.6
1	D	393	LYS	2.6
1	D	3	ALA	2.6
1	D	388	LEU	2.6
1	D	343	VAL	2.4
1	B	441	ASP	2.4
1	D	408	LYS	2.3
1	A	392	PRO	2.3
1	A	265[A]	LEU	2.3
1	D	451	ASP	2.3
1	B	443	PRO	2.3
1	D	385	SER	2.3
1	B	455	VAL	2.2
1	A	441	ASP	2.2
1	D	376	PRO	2.2
1	A	340[A]	GLN	2.2
1	D	440	TRP	2.2
1	D	394	ARG	2.1
1	A	388	LEU	2.1
1	D	441	ASP	2.1
1	B	392	PRO	2.1
1	D	455	VAL	2.1
1	A	393	LYS	2.1
1	C	344	SER	2.1
1	D	383	ALA	2.1
1	A	408	LYS	2.0
1	D	446	ARG	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. 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
3	HEC	A	600	43/43	0.95	0.13	23,29,33,38	0
3	HEC	B	600	43/43	0.96	0.12	20,24,27,29	0
3	HEC	D	600	43/43	0.96	0.10	22,26,28,29	0
3	HEC	C	600	43/43	0.97	0.07	14,17,22,24	0
2	CU	D	501	1/1	0.98	0.06	19,19,19,19	0
2	CU	A	501	1/1	0.99	0.07	18,18,18,18	0
2	CU	D	502	1/1	0.99	0.06	19,19,19,19	0
2	CU	A	502	1/1	0.99	0.07	15,15,15,15	0
2	CU	C	502	1/1	0.99	0.06	14,14,14,14	0
2	CU	B	501	1/1	0.99	0.06	17,17,17,17	0
2	CU	C	501	1/1	0.99	0.06	14,14,14,14	0
2	CU	B	502	1/1	1.00	0.07	16,16,16,16	0

## 6.5 Other polymers

There are no such residues in this entry.