



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:20 pm BST

PDB ID : 3SBQ  
Title : Pseudomonas stutzeri nitrous oxide reductase, P65 crystal form  
Authors : Pomowski, A.; Zumft, W.G.; Kroneck, P.M.H.; Einsle, O.  
Deposited on : 2011-06-06  
Resolution : 1.70 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

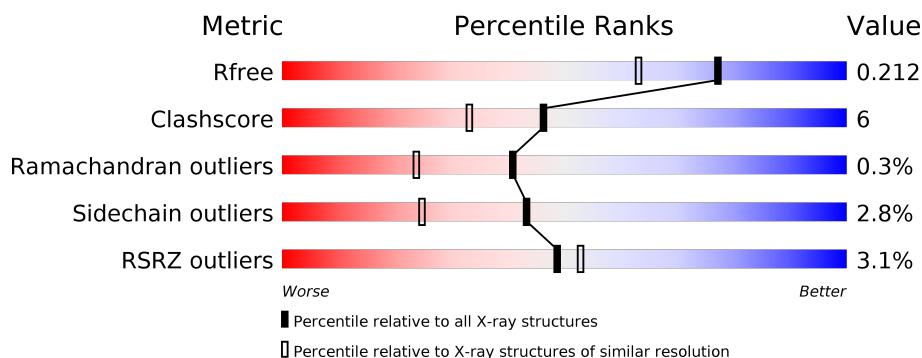
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 respectively. 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	638	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>9%</div> </div> </div>
1	B	638	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>9%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CL	B	704	-	-	X	-

## 2 Entry composition [i](#)

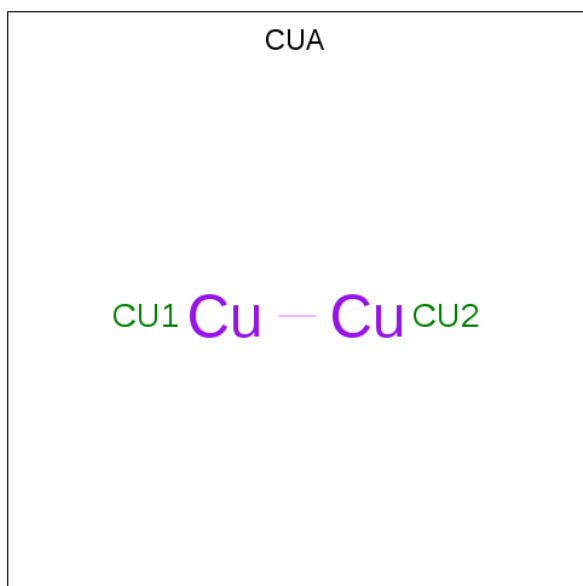
There are 8 unique types of molecules in this entry. The entry contains 9996 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nitrous-oxide reductase.

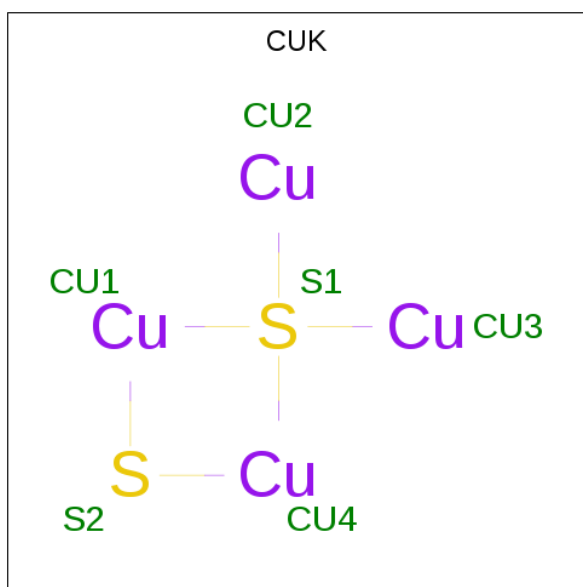
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	1	0
			4577	2893	788	864	32			
1	B	581	Total	C	N	O	S	0	5	0
			4609	2911	794	871	33			

- Molecule 2 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			2	2		
2	B	1	Total	Cu	0	0
			2	2		

- Molecule 3 is [4Cu:2S] cluster (three-letter code: CUK) (formula: Cu<sub>4</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Cu	S	0	0
			6	4	2		
3	B	1	Total	Cu	S	0	0
			6	4	2		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

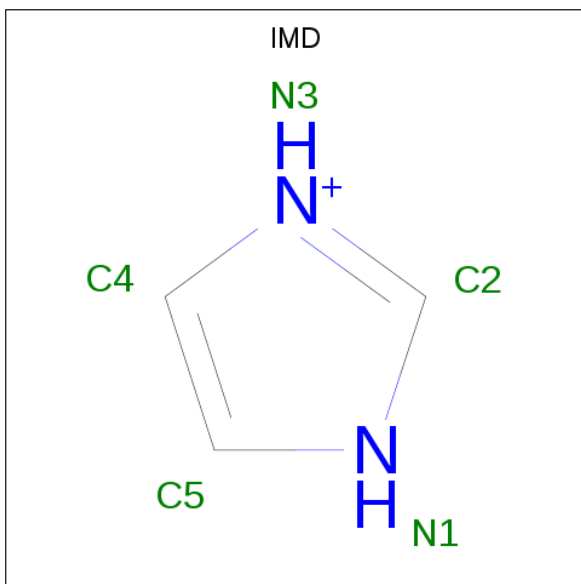
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	N	0	0
			5	3	2		

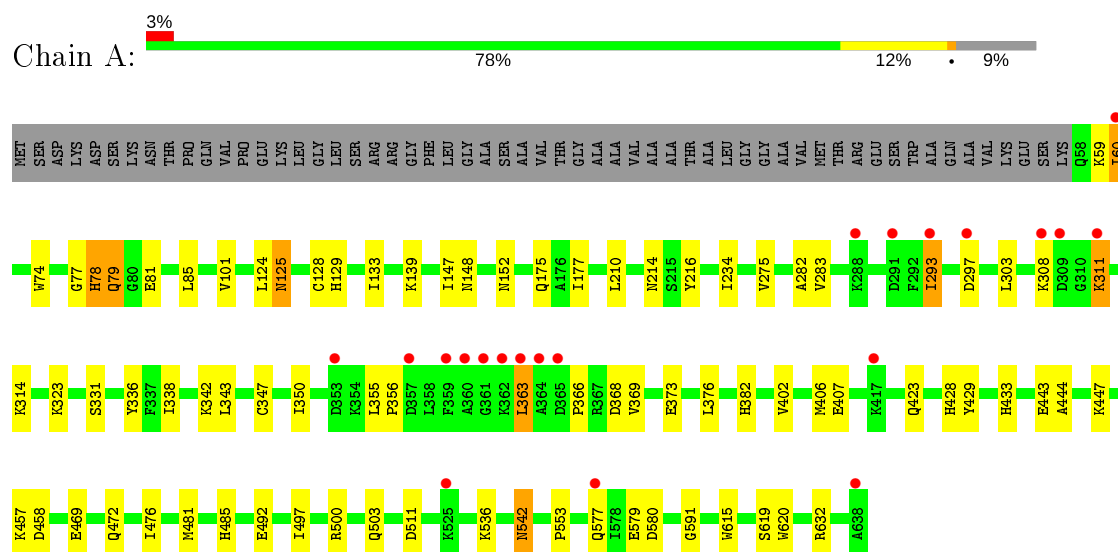
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	383	Total	O	0	0
			383	383		
8	B	400	Total	O	0	0
			400	400		

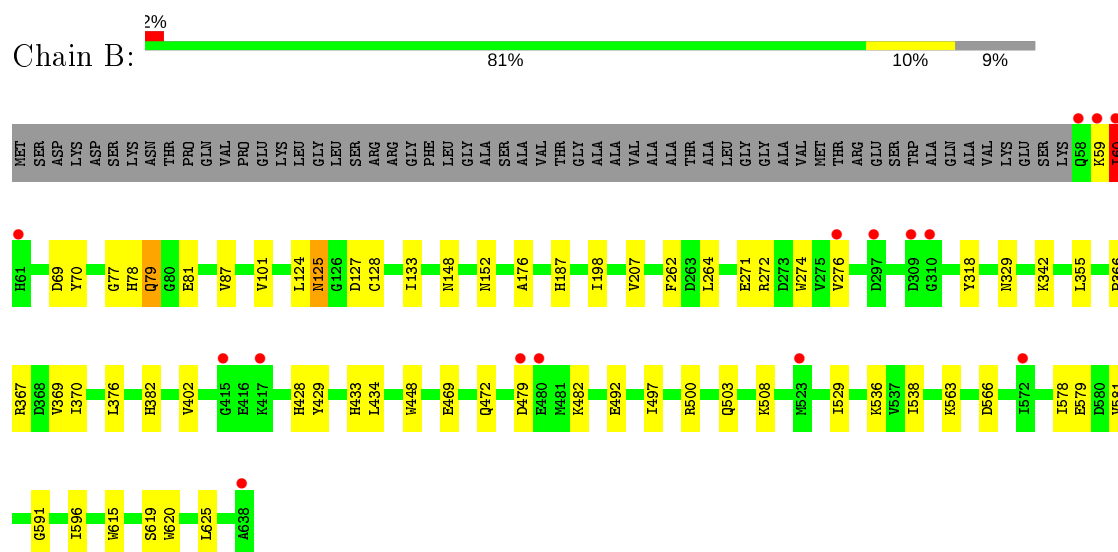
### 3 Residue-property plots [i](#)

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: Nitrous-oxide reductase



#### • Molecule 1: Nitrous-oxide reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.37 Å 70.37 Å 400.10 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.70 28.78 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-1.70) 98.6 (28.78-1.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 1.70 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.188 , 0.213 0.187 , 0.212	Depositor DCC
$R_{free}$ test set	6136 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.063 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9996	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IMD, CL, K, CUA, CUK, CA

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	0.54	0/4689	0.68	1/6349 (0.0%)
1	B	0.55	0/4722	0.67	0/6393
All	All	0.54	0/9411	0.67	1/12742 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	LEU	CA-CB-CG	5.18	127.22	115.30

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	4577	0	4442	71	0
1	B	4609	0	4463	52	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	3	0
7	B	5	0	5	3	0
8	A	383	0	0	5	1
8	B	400	0	0	2	0
All	All	9996	0	8910	115	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 6.

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:275:VAL:HG21	1:A:350:ILE:CD1	1.88	1.02
1:A:275:VAL:HG21	1:A:350:ILE:HD11	1.42	1.02
1:B:271[B]:GLU:HG3	8:B:914:HOH:O	1.71	0.89
1:A:469:GLU:HG3	1:A:492:GLU:HA	1.54	0.89
1:A:423:GLN:HE22	1:A:481:MET:H	1.21	0.89
1:A:275:VAL:CG2	1:A:350:ILE:HD11	2.04	0.88
1:B:469:GLU:HG3	1:B:492:GLU:HA	1.56	0.87
1:A:125:ASN:HD21	1:B:591:GLY:HA2	1.41	0.85
1:A:591:GLY:HA2	1:B:125:ASN:HD21	1.42	0.84
1:B:133:ILE:HG13	1:B:497:ILE:HD12	1.64	0.79
1:A:133:ILE:HG13	1:A:497:ILE:HD12	1.67	0.77
1:A:428:HIS:H	1:A:472:GLN:HE22	1.32	0.76
1:B:382[B]:HIS:CE1	6:B:704:CL:CL	2.75	0.76
1:B:578:ILE:O	1:B:581:VAL:HG12	1.88	0.74
1:B:59:LYS:O	1:B:60:ILE:HG22	1.89	0.73
1:A:129:HIS:H	1:A:148:ASN:HD21	1.36	0.72
1:A:125:ASN:ND2	1:B:591:GLY:HA2	2.08	0.68
1:A:366:PRO:O	1:A:369:VAL:HG22	1.95	0.66
1:A:275:VAL:CG2	1:A:350:ILE:CD1	2.67	0.65
1:A:275:VAL:HG21	1:A:350:ILE:HD12	1.80	0.63
1:A:283:VAL:HG13	1:A:303:LEU:HD12	1.81	0.63
1:A:128:CYS:HB2	1:A:147:ILE:HG12	1.81	0.62
1:B:382[B]:HIS:HE1	6:B:704:CL:CL	2.18	0.62
1:B:329:ASN:HD21	1:B:382[B]:HIS:CE1	2.19	0.60
1:A:331:SER:HB3	1:A:406:MET:HE3	1.83	0.60
1:B:382[B]:HIS:HD2	1:B:434:LEU:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD13	8:A:662:HOH:O	2.02	0.59
1:A:283:VAL:HG13	1:A:303:LEU:CD1	2.32	0.59
1:A:632:ARG:HD2	1:B:262:PHE:HB2	1.85	0.59
1:B:128:CYS:HB3	1:B:148:ASN:O	2.03	0.58
1:B:428:HIS:H	1:B:472:GLN:HE22	1.50	0.58
1:B:382[A]:HIS:NE2	1:B:433:HIS:CD2	2.72	0.58
1:A:591:GLY:HA2	1:B:125:ASN:ND2	2.16	0.58
1:B:274:TRP:CD1	1:B:276:VAL:HG23	2.38	0.57
1:A:79:GLN:HE22	1:A:81:GLU:CG	2.18	0.57
1:A:336:TYR:HD2	1:A:406:MET:CE	2.18	0.57
1:A:428:HIS:H	1:A:472:GLN:NE2	2.02	0.57
1:B:382[A]:HIS:CE1	1:B:433:HIS:NE2	2.73	0.56
1:B:79:GLN:HE22	1:B:81:GLU:CG	2.19	0.55
1:A:423:GLN:HE22	1:A:481:MET:N	1.99	0.55
1:B:133:ILE:HG13	1:B:497:ILE:CD1	2.34	0.55
1:A:338:ILE:HD11	1:A:406:MET:HE3	1.89	0.54
1:B:78:HIS:HD2	1:B:127:ASP:OD1	1.90	0.54
1:A:632:ARG:HD3	8:A:983:HOH:O	2.07	0.54
1:B:59:LYS:NZ	1:B:448:TRP:HE1	2.06	0.53
1:A:125:ASN:ND2	1:A:152:ASN:HD21	2.06	0.53
1:B:276:VAL:HG22	1:B:318:TYR:CD2	2.44	0.53
1:B:382[A]:HIS:CD2	1:B:433:HIS:CD2	2.97	0.53
1:B:469:GLU:CG	1:B:492:GLU:HA	2.34	0.53
1:B:271[A]:GLU:HG2	1:B:272:ARG:HG3	1.90	0.53
1:B:198:ILE:H	7:B:639:IMD:HN1	1.57	0.52
1:A:323:LYS:HG3	1:A:343:LEU:HB2	1.92	0.52
1:A:59:LYS:O	1:A:60:ILE:CG2	2.58	0.52
1:B:500:ARG:HB2	1:B:503:GLN:HG3	1.92	0.52
1:A:129:HIS:N	1:A:148:ASN:HD21	2.07	0.51
1:A:59:LYS:O	1:A:60:ILE:HG23	2.11	0.51
1:A:148:ASN:HD22	1:A:148:ASN:H	1.59	0.51
1:B:274:TRP:CD1	1:B:276:VAL:CG2	2.94	0.51
1:B:382[A]:HIS:NE2	1:B:433:HIS:NE2	2.58	0.50
1:A:125:ASN:HD21	1:A:152:ASN:HD21	1.58	0.50
1:B:433:HIS:HD2	3:B:702:CUK:S2	2.35	0.50
1:B:59:LYS:HE3	1:B:69:ASP:OD2	2.10	0.50
1:A:129:HIS:H	1:A:148:ASN:ND2	2.08	0.50
1:A:214:ASN:ND2	8:A:727:HOH:O	2.44	0.50
1:A:336:TYR:HD2	1:A:406:MET:HE1	1.77	0.50
1:B:508:LYS:HD3	1:B:579:GLU:OE1	2.11	0.50
1:A:77:GLY:HA2	1:A:128:CYS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:HIS:CD2	1:A:433:HIS:HA	2.48	0.49
1:A:148:ASN:HB2	1:A:177:ILE:HG22	1.95	0.49
1:B:428:HIS:HA	1:B:429:TYR:CG	2.48	0.48
1:A:553:PRO:HG2	1:B:264:LEU:HD11	1.96	0.47
1:A:175:GLN:HE22	1:B:615:TRP:H	1.61	0.47
1:A:615:TRP:CH2	7:B:639:IMD:H5	2.48	0.47
1:A:101:VAL:HG21	1:A:124:LEU:HD22	1.95	0.47
1:A:338:ILE:HD11	1:A:406:MET:CE	2.45	0.46
1:A:382:HIS:CE1	1:A:433:HIS:CE1	3.04	0.46
1:A:308:LYS:O	1:A:311:LYS:HG2	2.16	0.46
1:A:429:TYR:CD2	1:A:457:LYS:HD2	2.51	0.46
1:A:336:TYR:CD2	1:A:406:MET:CE	2.97	0.46
1:A:443:GLU:O	1:A:444:ALA:C	2.54	0.46
1:B:101:VAL:HG21	1:B:124:LEU:HD22	1.98	0.45
1:B:366:PRO:O	1:B:369:VAL:HG22	2.17	0.45
1:A:293:ILE:HG22	8:A:1004:HOH:O	2.17	0.45
1:A:282:ALA:HB1	1:A:314:LYS:HD2	1.99	0.45
1:B:70:TYR:HB2	1:B:87:VAL:HB	1.98	0.44
1:A:619:SER:O	1:B:78:HIS:NE2	2.51	0.44
1:A:469:GLU:CG	1:A:492:GLU:HA	2.38	0.44
1:B:428:HIS:H	1:B:472:GLN:NE2	2.15	0.44
1:A:79:GLN:HE22	1:A:81:GLU:HG2	1.82	0.44
1:B:77:GLY:HA2	1:B:128:CYS:O	2.17	0.44
1:A:376:LEU:HB3	1:A:402:VAL:HG11	2.00	0.43
1:A:355:LEU:N	1:A:356:PRO:CD	2.81	0.43
1:A:363:LEU:HD13	1:A:368:ASP:HB2	2.01	0.43
1:A:347:CYS:O	1:A:373:GLU:HA	2.19	0.43
7:B:639:IMD:H4	8:B:719:HOH:O	2.19	0.43
1:A:78:HIS:NE2	1:B:619:SER:O	2.51	0.42
1:A:216:TYR:CD1	1:A:234:ILE:HG23	2.53	0.42
1:A:139:LYS:HG2	1:A:443:GLU:HG3	2.01	0.42
1:B:382[B]:HIS:ND1	6:B:704:CL:CL	2.88	0.42
1:A:485:HIS:ND1	8:A:653:HOH:O	2.05	0.42
1:A:500:ARG:HB2	1:A:503:GLN:HG3	2.03	0.41
1:A:78:HIS:CE1	1:A:492:GLU:HB3	2.55	0.41
1:A:579:GLU:O	1:A:580:ASP:CB	2.68	0.41
1:A:542:ASN:HD22	1:A:542:ASN:C	2.23	0.41
1:A:323:LYS:CG	1:A:343:LEU:HB2	2.50	0.41
1:A:428:HIS:HA	1:A:429:TYR:CG	2.56	0.41
1:A:476:ILE:HG22	1:A:481:MET:HG2	2.03	0.41
1:B:125:ASN:ND2	1:B:152:ASN:HD21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ARG:HD2	1:B:370:ILE:HD12	2.01	0.41
1:B:376:LEU:HB3	1:B:402:VAL:HG11	2.03	0.41
1:B:79:GLN:HB3	1:B:79:GLN:HE21	1.59	0.41
1:B:563:LYS:HE3	1:B:566:ASP:OD1	2.20	0.41
1:B:367:ARG:NH1	1:B:370:ILE:HD13	2.35	0.41
1:B:529:ILE:CD1	1:B:536:LYS:HD2	2.50	0.41
1:A:79:GLN:HE21	1:A:79:GLN:HB3	1.72	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)
1:B:187:HIS:NE2	8:A:1002:HOH:O[1_445]	1.99	0.21

## 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	580/638 (91%)	550 (95%)	29 (5%)	1 (0%)	47	30
1	B	584/638 (92%)	558 (96%)	23 (4%)	3 (0%)	29	13
All	All	1164/1276 (91%)	1108 (95%)	52 (4%)	4 (0%)	41	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	LYS
1	B	342	LYS
1	B	176	ALA
1	B	60	ILE

### 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	497/537 (93%)	480 (97%)	17 (3%)	37	18
1	B	501/537 (93%)	490 (98%)	11 (2%)	52	34
All	All	998/1074 (93%)	970 (97%)	28 (3%)	43	25

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	74	TRP
1	A	78	HIS
1	A	79	GLN
1	A	125	ASN
1	A	293	ILE
1	A	297	ASP
1	A	311	LYS
1	A	363	LEU
1	A	407	GLU
1	A	447	LYS
1	A	458	ASP
1	A	511	ASP
1	A	536	LYS
1	A	542	ASN
1	A	577	GLN
1	A	620	TRP
1	B	60	ILE
1	B	79	GLN
1	B	125	ASN
1	B	207	VAL
1	B	355	LEU
1	B	479	ASP
1	B	482	LYS
1	B	538	ILE
1	B	596	ILE
1	B	620	TRP

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Mol	Chain	Res	Type
1	B	625	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	78	HIS
1	A	79	GLN
1	A	111	ASN
1	A	125	ASN
1	A	129	HIS
1	A	148	ASN
1	A	175	GLN
1	A	201	HIS
1	A	423	GLN
1	A	472	GLN
1	A	542	ASN
1	A	558	GLN
1	A	577	GLN
1	B	78	HIS
1	B	79	GLN
1	B	111	ASN
1	B	125	ASN
1	B	201	HIS
1	B	211	GLN
1	B	214	ASN
1	B	430	GLN
1	B	467	HIS
1	B	472	GLN
1	B	577	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

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	IMD	B	639	-	3,5,5	0.39	0	4,5,5	0.62	0
2	CUA	A	701	1	0,1,1	0.00	-	-		
2	CUA	B	701	1	0,1,1	0.00	-	-		
3	CUK	B	702	1	0,6,6	0.00	-	-		
3	CUK	A	702	1	0,6,6	0.00	-	-		

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	IMD	B	639	-	-	-	0/1/1/1
3	CUK	B	702	1	-	-	0/1/1/1
3	CUK	A	702	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	639	IMD	3	0
3	B	702	CUK	1	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	581/638 (91%)	0.10	21 (3%)	42 47	17, 27, 41, 49	0
1	B	581/638 (91%)	0.03	15 (2%)	56 60	17, 26, 39, 47	0
All	All	1162/1276 (91%)	0.07	36 (3%)	49 53	17, 27, 40, 49	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	ALA	8.1
1	A	638	ALA	6.9
1	B	638	ALA	6.4
1	A	360	ALA	4.3
1	A	362	LYS	4.0
1	B	59	LYS	3.5
1	A	365	ASP	3.5
1	A	297	ASP	3.5
1	A	311	LYS	3.2
1	A	309	ASP	3.1
1	A	363	LEU	3.0
1	B	310	GLY	2.8
1	A	353	ASP	2.8
1	A	291	ASP	2.8
1	B	417	LYS	2.7
1	A	293	ILE	2.6
1	B	60	ILE	2.6
1	B	297	ASP	2.6
1	A	577	GLN	2.6
1	A	60	ILE	2.6
1	A	417	LYS	2.6
1	A	357	ASP	2.6
1	A	288	LYS	2.5
1	B	480	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	525	LYS	2.4
1	A	308	LYS	2.4
1	B	276	VAL	2.3
1	A	361	GLY	2.3
1	B	58	GLN	2.3
1	B	415	GLY	2.2
1	B	309	ASP	2.2
1	B	479	ASP	2.1
1	B	61	HIS	2.1
1	B	572	ILE	2.1
1	B	523[A]	MET	2.1
1	A	359	PHE	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
6	CL	B	704	1/1	0.94	0.09	34,34,34,34	0
3	CUK	B	702	6/6	0.94	0.12	39,41,44,45	6
7	IMD	B	639	5/5	0.95	0.10	42,42,43,43	0
4	K	A	705	1/1	0.97	0.08	35,35,35,35	0
3	CUK	A	702	6/6	0.97	0.07	33,38,43,43	6
2	CUA	B	701	2/2	0.98	0.05	29,29,29,32	0
5	CA	B	703	1/1	0.99	0.02	23,23,23,23	0
5	CA	A	703	1/1	0.99	0.02	27,27,27,27	0
2	CUA	A	701	2/2	0.99	0.03	28,28,28,29	0
4	K	B	705	1/1	0.99	0.11	37,37,37,37	0
6	CL	A	704	1/1	1.00	0.02	33,33,33,33	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.