



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:00 PM GMT

PDB ID : 3SBP  
Title : Pseudomonas stutzeri nitrous oxide reductase, P1 crystal form  
Authors : Pomowski, A.; Zumft, W.G.; Kroneck, P.M.H.; Einsle, O.  
Deposited on : 2011-06-06  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

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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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

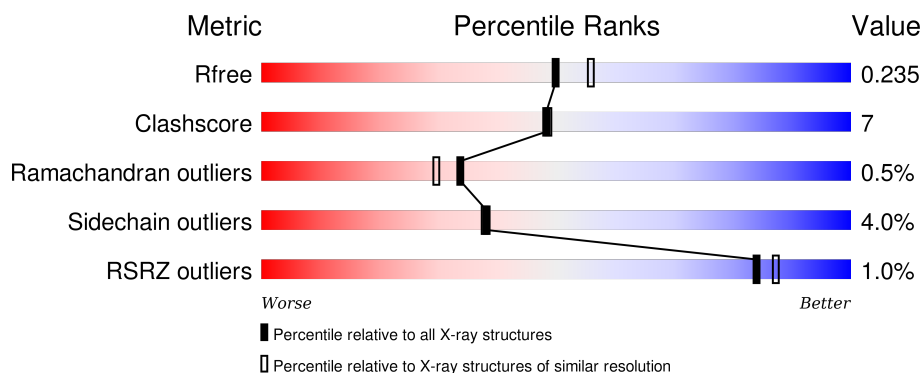
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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  $\geq 3$ , 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	638	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	638	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	638	<div> <div></div> <div> <div></div> <div>77%</div> <div>12%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	638	<div> <div></div> <div> <div></div> <div>78%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>
1	E	638	<div> <div></div> <div> <div></div> <div>79%</div> <div>11%</div> <div>•</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	638	 79%10% • 9%
1	G	638	 79%12% • 8%
1	H	638	 77%13% • 9%

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
7	IMD	D	639	-	-	-	X
7	IMD	F	639	-	-	-	X
7	IMD	H	639	-	-	X	-

## 2 Entry composition

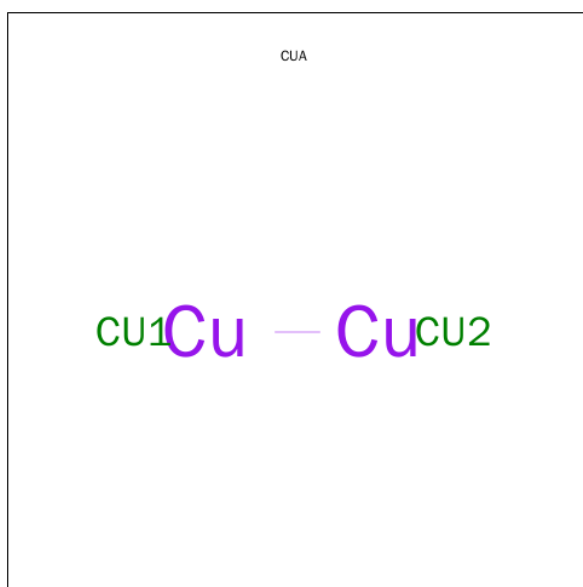
There are 8 unique types of molecules in this entry. The entry contains 39843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

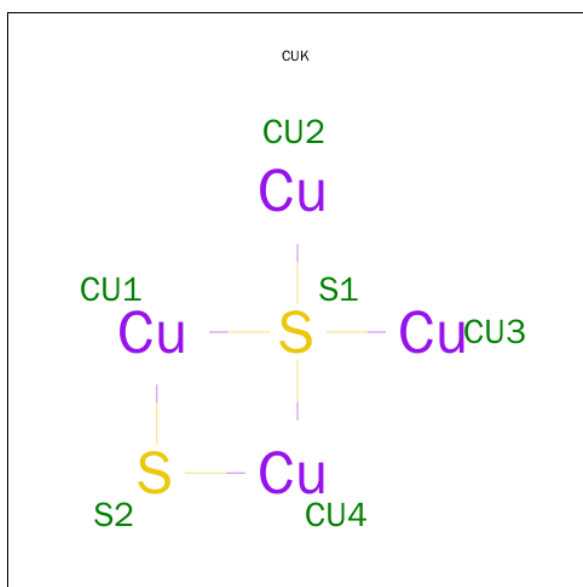
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	1	0
			4573	2891	788	862	32			
1	B	581	Total	C	N	O	S	0	3	0
			4592	2902	792	866	32			
1	C	581	Total	C	N	O	S	0	3	0
			4590	2900	790	868	32			
1	D	588	Total	C	N	O	S	0	2	0
			4636	2929	799	876	32			
1	E	581	Total	C	N	O	S	0	1	0
			4575	2892	788	863	32			
1	F	581	Total	C	N	O	S	0	3	0
			4593	2902	790	869	32			
1	G	585	Total	C	N	O	S	0	1	0
			4606	2911	794	869	32			
1	H	581	Total	C	N	O	S	0	3	0
			4590	2900	790	868	32			

- 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		
2	C	1	Total	Cu	0	0
			2	2		
2	D	1	Total	Cu	0	0
			2	2		
2	E	1	Total	Cu	0	0
			2	2		
2	F	1	Total	Cu	0	0
			2	2		
2	G	1	Total	Cu	0	0
			2	2		
2	H	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		
3	C	1	Total	Cu	S	0	0
			6	4	2		
3	D	1	Total	Cu	S	0	0
			6	4	2		
3	E	1	Total	Cu	S	0	0
			6	4	2		
3	F	1	Total	Cu	S	0	0
			6	4	2		
3	G	1	Total	Cu	S	0	0
			6	4	2		
3	H	1	Total	Cu	S	0	0
			6	4	2		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Ca	0	0
			1	1		
4	D	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	H	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0
4	A	1	Total 1	Ca 1	0	0
4	F	1	Total 1	Ca 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total 1	Cl 1	0	0
5	D	1	Total 1	Cl 1	0	0
5	E	1	Total 1	Cl 1	0	0
5	H	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	C	1	Total 1	Cl 1	0	0
5	A	1	Total 1	Cl 1	0	0
5	F	1	Total 1	Cl 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

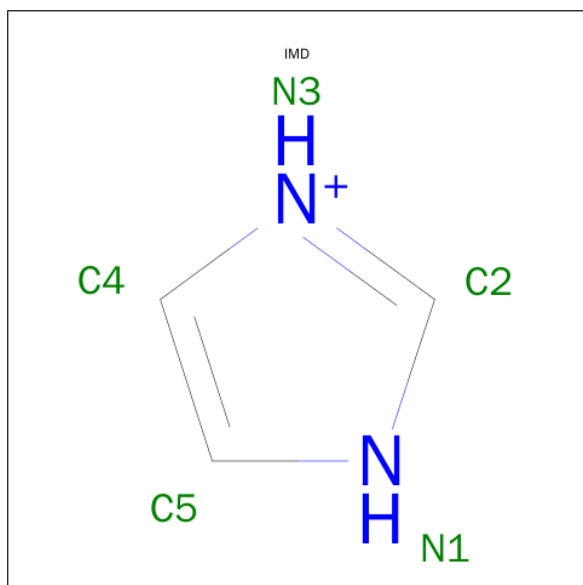
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	E	1	Total 1	K 1	0	0
6	H	1	Total 1	K 1	0	0
6	B	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	K	0	0
			1	1		
6	A	1	Total	K	0	0
			1	1		
6	F	1	Total	K	0	0
			1	1		

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



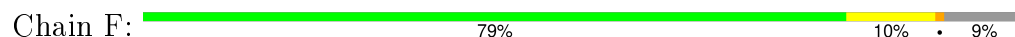
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	N	0	0
			5	3	2		
7	E	1	Total	C	N	0	0
			5	3	2		
7	E	1	Total	C	N	0	0
			5	3	2		
7	F	1	Total	C	N	0	0
			5	3	2		
7	G	1	Total	C	N	0	0
			5	3	2		
7	H	1	Total	C	N	0	0
			5	3	2		

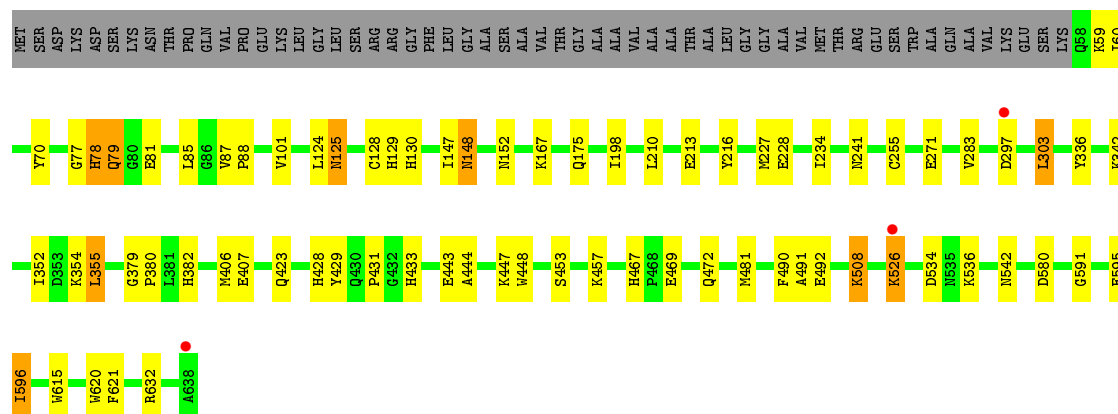
- Molecule 8 is water.



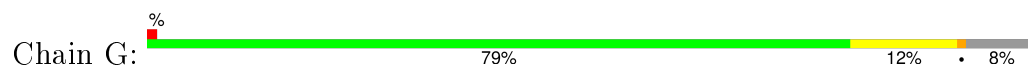
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	232	Total 232	O 232	0	0
8	B	218	Total 218	O 218	0	0
8	C	409	Total 409	O 409	0	0
8	D	419	Total 419	O 419	0	0
8	E	439	Total 439	O 439	0	0
8	F	446	Total 446	O 446	0	0
8	G	406	Total 406	O 406	0	0
8	H	401	Total 401	O 401	0	0



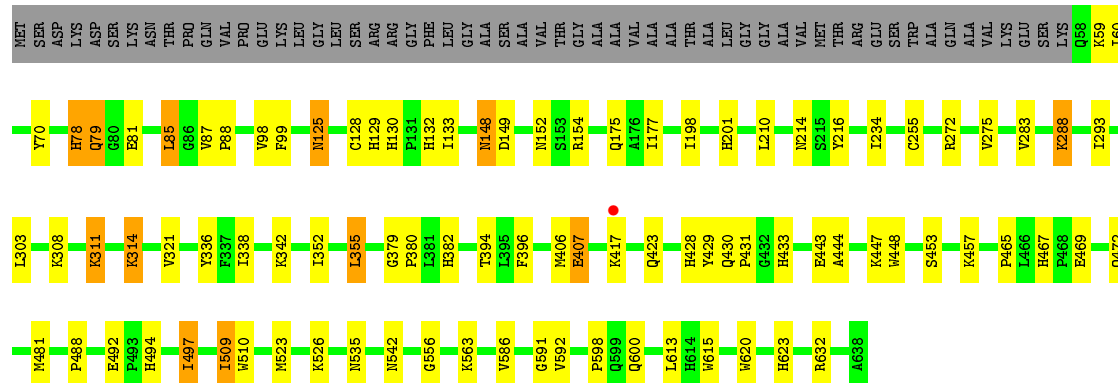
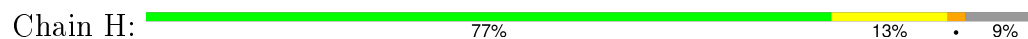




• Molecule 1: Nitrous-oxide reductase



• Molecule 1: Nitrous-oxide reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.89Å 106.70Å 131.14Å 111.34° 107.33° 90.74°	Depositor
Resolution (Å)	46.02 – 2.10 45.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.7 (46.02-2.10) 82.7 (45.81-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.177 , 0.236 0.178 , 0.235	Depositor DCC
$R_{free}$ test set	12842 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.2	EDS
Estimated twinning fraction	0.013 for -h,k,-k-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 255616 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	39843	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.44	0/4685	0.61	1/6345 (0.0%)
1	B	0.45	0/4705	0.61	1/6372 (0.0%)
1	C	0.53	0/4702	0.66	1/6368 (0.0%)
1	D	0.52	0/4748	0.66	1/6428 (0.0%)
1	E	0.53	0/4687	0.68	2/6348 (0.0%)
1	F	0.54	0/4705	0.66	1/6372 (0.0%)
1	G	0.52	0/4718	0.66	0/6387
1	H	0.53	0/4702	0.65	1/6368 (0.0%)
All	All	0.51	0/37652	0.65	8/50988 (0.0%)

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	C	0	1
1	D	0	1
1	G	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	LEU	CA-CB-CG	7.97	133.64	115.30
1	H	85	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	85	LEU	CA-CB-CG	5.71	128.43	115.30
1	D	85	LEU	CA-CB-CG	5.66	128.32	115.30
1	F	85	LEU	CA-CB-CG	5.49	127.92	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	274	TRP	Peptide
1	D	58	GLN	Peptide
1	G	58	GLN	Peptide

## 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	4573	0	4441	71	0
1	B	4592	0	4452	80	0
1	C	4590	0	4449	74	0
1	D	4636	0	4505	74	0
1	E	4575	0	4440	70	0
1	F	4593	0	4450	61	0
1	G	4606	0	4478	65	0
1	H	4590	0	4449	77	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
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
3	G	6	0	0	0	0
3	H	6	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	D	5	0	5	2	0
7	E	10	0	10	4	0
7	F	5	0	5	3	0
7	G	5	0	5	0	0
7	H	5	0	5	4	0
8	A	232	0	0	5	0
8	B	218	0	0	4	0
8	C	409	0	0	6	0
8	D	419	0	0	13	0
8	E	439	0	0	10	0
8	F	446	0	0	10	0
8	G	406	0	0	10	0
8	H	401	0	0	12	0
All	All	39843	0	35694	532	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 7.

The worst 5 of 532 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:H:338:ILE:HD11	1:H:406:MET:CE	1.89	1.03
8:D:2328:HOH:O	1:E:542:ASN:HB3	1.60	1.02
1:H:423:GLN:HE22	1:H:481:MET:H	1.08	1.01
1:E:423:GLN:HE22	1:E:481:MET:H	1.09	0.97
1:C:338:ILE:HD11	1:C:406:MET:HE3	1.45	0.96

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	580/638 (91%)	544 (94%)	30 (5%)	6 (1%)	19	13
1	B	582/638 (91%)	547 (94%)	32 (6%)	3 (0%)	34	30
1	C	582/638 (91%)	557 (96%)	22 (4%)	3 (0%)	34	30
1	D	588/638 (92%)	557 (95%)	29 (5%)	2 (0%)	46	45
1	E	580/638 (91%)	555 (96%)	24 (4%)	1 (0%)	52	53
1	F	582/638 (91%)	556 (96%)	25 (4%)	1 (0%)	52	53
1	G	584/638 (92%)	551 (94%)	30 (5%)	3 (0%)	34	30
1	H	582/638 (91%)	554 (95%)	25 (4%)	3 (0%)	34	30
All	All	4660/5104 (91%)	4421 (95%)	217 (5%)	22 (0%)	34	30

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	LYS
1	B	60	ILE
1	C	59	LYS
1	A	269	ARG
1	A	308	LYS

### 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%)	472 (95%)	25 (5%)	30	27
1	B	499/537 (93%)	478 (96%)	21 (4%)	36	35
1	C	499/537 (93%)	478 (96%)	21 (4%)	36	35
1	D	504/537 (94%)	487 (97%)	17 (3%)	44	45
1	E	497/537 (93%)	482 (97%)	15 (3%)	48	51
1	F	499/537 (93%)	480 (96%)	19 (4%)	40	40
1	G	501/537 (93%)	479 (96%)	22 (4%)	35	33
1	H	499/537 (93%)	479 (96%)	20 (4%)	38	38
All	All	3995/4296 (93%)	3835 (96%)	160 (4%)	38	38

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	225	GLU
1	E	213	GLU
1	H	255	CYS
1	D	293	ILE
1	D	542	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 104 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	201	HIS
1	E	175	GLN
1	H	148	ASN
1	D	214	ASN
1	D	542	ASN

### 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 46 ligands modelled in this entry, 24 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CUA	A	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	A	702	1	0,6,6	0.00	-	0,9,9	0.00	-
2	CUA	B	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	B	702	1	0,6,6	0.00	-	0,9,9	0.00	-
2	CUA	C	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	C	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	D	639	-	3,5,5	0.53	0	4,5,5	0.55	0
2	CUA	D	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	D	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	E	639	-	3,5,5	0.55	0	4,5,5	0.46	0
7	IMD	E	640	-	3,5,5	0.51	0	4,5,5	0.42	0
2	CUA	E	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	E	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	F	639	-	3,5,5	0.47	0	4,5,5	0.72	0
2	CUA	F	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	F	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	G	639	-	3,5,5	0.60	0	4,5,5	0.60	0
2	CUA	G	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	G	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	H	639	-	3,5,5	0.45	0	4,5,5	0.54	0
2	CUA	H	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	H	702	1	0,6,6	0.00	-	0,9,9	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
2	CUA	A	701	1	-	0/0/0/0	0/0/0/0
3	CUK	A	702	1	-	0/0/8/8	0/1/1/1
2	CUA	B	701	1	-	0/0/0/0	0/0/0/0
3	CUK	B	702	1	-	0/0/8/8	0/1/1/1
2	CUA	C	701	1	-	0/0/0/0	0/0/0/0
3	CUK	C	702	1	-	0/0/8/8	0/1/1/1
7	IMD	D	639	-	-	0/0/0/0	0/1/1/1
2	CUA	D	701	1	-	0/0/0/0	0/0/0/0
3	CUK	D	702	1	-	0/0/8/8	0/1/1/1
7	IMD	E	639	-	-	0/0/0/0	0/1/1/1
7	IMD	E	640	-	-	0/0/0/0	0/1/1/1
2	CUA	E	701	1	-	0/0/0/0	0/0/0/0
3	CUK	E	702	1	-	0/0/8/8	0/1/1/1
7	IMD	F	639	-	-	0/0/0/0	0/1/1/1
2	CUA	F	701	1	-	0/0/0/0	0/0/0/0
3	CUK	F	702	1	-	0/0/8/8	0/1/1/1
7	IMD	G	639	-	-	0/0/0/0	0/1/1/1
2	CUA	G	701	1	-	0/0/0/0	0/0/0/0
3	CUK	G	702	1	-	0/0/8/8	0/1/1/1
7	IMD	H	639	-	-	0/0/0/0	0/1/1/1
2	CUA	H	701	1	-	0/0/0/0	0/0/0/0
3	CUK	H	702	1	-	0/0/8/8	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.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	639	IMD	2	0
7	E	639	IMD	2	0
7	E	640	IMD	2	0
7	F	639	IMD	3	0
7	H	639	IMD	4	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%)	0.03	19 (3%) 50 59	20, 33, 56, 70	0
1	B	581/638 (91%)	0.05	13 (2%) 65 71	20, 33, 51, 62	0
1	C	581/638 (91%)	-0.44	1 (0%) 95 96	10, 18, 31, 40	0
1	D	588/638 (92%)	-0.33	3 (0%) 91 93	9, 22, 36, 44	0
1	E	581/638 (91%)	-0.42	1 (0%) 95 96	8, 17, 29, 37	0
1	F	581/638 (91%)	-0.39	3 (0%) 91 93	10, 17, 31, 40	0
1	G	585/638 (91%)	-0.31	4 (0%) 89 91	10, 22, 39, 50	0
1	H	581/638 (91%)	-0.37	1 (0%) 95 96	11, 20, 35, 45	0
All	All	4659/5104 (91%)	-0.27	45 (0%) 84 87	8, 22, 43, 70	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	638	ALA	4.5
1	A	310	GLY	4.2
1	B	638	ALA	3.4
1	B	297	ASP	3.4
1	B	310	GLY	3.3

### 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, 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	IMD	D	639	5/5	0.89	0.15	4.63	46,46,47,47	0
7	IMD	F	639	5/5	0.91	0.16	3.85	47,47,48,48	0
7	IMD	E	640	5/5	0.97	0.12	1.99	24,24,25,25	0
7	IMD	G	639	5/5	0.93	0.15	0.84	45,45,45,46	0
3	CUK	B	702	6/6	0.84	0.13	-0.02	57,61,62,62	6
5	CL	B	704	1/1	0.98	0.11	-0.24	50,50,50,50	0
7	IMD	H	639	5/5	0.98	0.08	-0.87	22,22,23,24	0
6	K	G	705	1/1	0.94	0.09	-1.01	44,44,44,44	0
4	CA	C	703	1/1	1.00	0.08	-1.08	15,15,15,15	0
5	CL	C	704	1/1	0.99	0.07	-1.14	26,26,26,26	0
5	CL	E	704	1/1	1.00	0.07	-1.15	23,23,23,23	0
5	CL	G	704	1/1	0.99	0.09	-1.21	29,29,29,29	0
5	CL	F	704	1/1	0.99	0.07	-1.23	24,24,24,24	0
4	CA	H	703	1/1	0.99	0.07	-1.54	15,15,15,15	0
4	CA	D	703	1/1	0.98	0.06	-1.56	25,25,25,25	0
3	CUK	H	702	6/6	0.95	0.09	-1.58	34,37,39,40	6
4	CA	A	703	1/1	0.90	0.09	-1.63	47,47,47,47	0
3	CUK	D	702	6/6	0.98	0.06	-1.69	27,34,36,38	6
3	CUK	E	702	6/6	0.96	0.07	-1.75	31,37,40,41	6
4	CA	E	703	1/1	0.99	0.06	-1.76	18,18,18,18	0
4	CA	F	703	1/1	1.00	0.04	-1.87	17,17,17,17	0
3	CUK	F	702	6/6	0.95	0.07	-1.89	26,32,34,36	6
4	CA	B	703	1/1	0.99	0.05	-2.00	27,27,27,27	0
3	CUK	G	702	6/6	0.94	0.07	-2.20	34,41,44,45	6
3	CUK	A	702	6/6	0.95	0.07	-2.27	49,53,53,54	6
6	K	C	705	1/1	0.89	0.08	-2.28	41,41,41,41	0
6	K	A	705	1/1	0.86	0.10	-2.33	54,54,54,54	0
4	CA	G	703	1/1	0.99	0.06	-2.41	26,26,26,26	0
5	CL	A	704	1/1	0.96	0.06	-2.49	46,46,46,46	0
3	CUK	C	702	6/6	0.97	0.06	-2.60	29,36,38,39	6
5	CL	H	704	1/1	0.99	0.04	-2.82	29,29,29,29	0
2	CUA	B	701	2/2	0.96	0.04	-2.98	52,52,52,54	0
6	K	D	705	1/1	0.95	0.05	-3.05	31,31,31,31	0
6	K	B	705	1/1	0.97	0.04	-3.24	48,48,48,48	0
2	CUA	G	701	2/2	0.98	0.06	-3.50	19,19,19,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	K	H	705	1/1	0.94	0.07	-3.70	37,37,37,37	0
2	CUA	F	701	2/2	0.98	0.06	-3.76	22,22,22,33	0
2	CUA	C	701	2/2	0.98	0.04	-3.88	27,27,27,33	0
2	CUA	E	701	2/2	0.99	0.04	-4.02	18,18,18,24	0
6	K	E	705	1/1	0.89	0.08	-4.08	46,46,46,46	0
2	CUA	A	701	2/2	0.96	0.04	-4.12	31,31,31,34	0
5	CL	D	704	1/1	0.99	0.03	-4.58	25,25,25,25	0
6	K	F	705	1/1	0.99	0.03	-5.54	26,26,26,26	0
2	CUA	H	701	2/2	0.99	0.03	-6.18	33,33,33,35	0
2	CUA	D	701	2/2	0.99	0.04	-9.65	21,21,21,23	0
7	IMD	E	639	5/5	0.97	0.12	-	37,37,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.