



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 3SBP / pdb_00003sbp
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

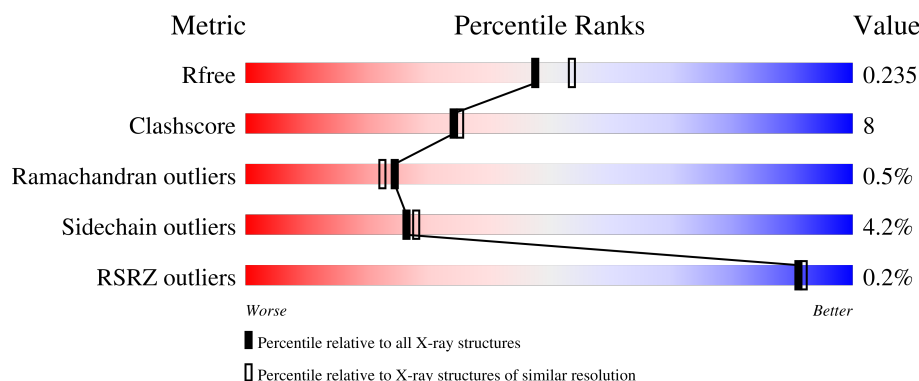
1 Overall quality at a glance

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	638	
1	C	638	
1	D	638	
1	E	638	

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Mol	Chain	Length	Quality of chain
1	F	638	 79% 11% • 9%
1	G	638	 78% 12% • 8%
1	H	638	 76% 14% • 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	H	639	-	-	X	-

2 Entry composition

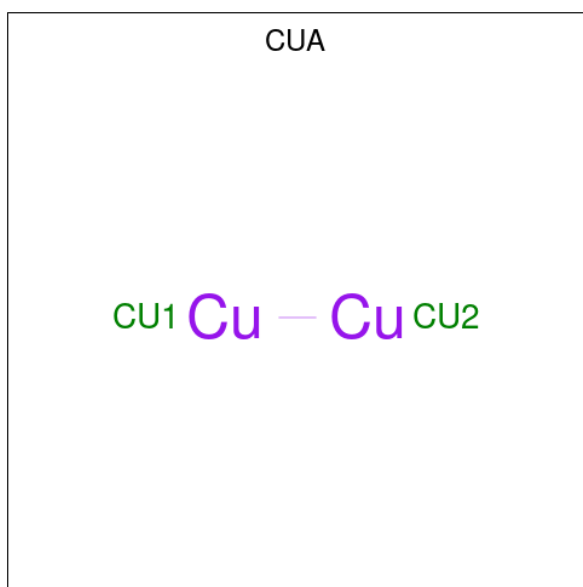
There are 8 unique types of molecules in this entry. The entry contains 39843 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

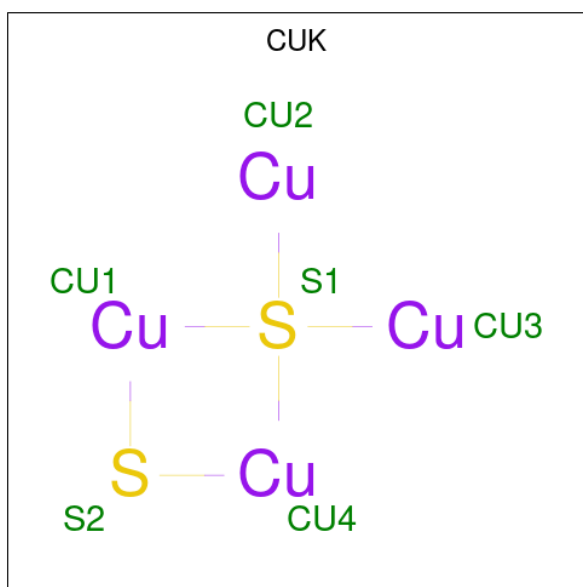
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	1	0
			4573	2891	788	862	32			
1	B	581	Total	C	N	O	S	0	3	0
			4592	2902	792	866	32			
1	C	581	Total	C	N	O	S	0	3	0
			4590	2900	790	868	32			
1	D	588	Total	C	N	O	S	0	2	0
			4636	2929	799	876	32			
1	E	581	Total	C	N	O	S	0	1	0
			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 (CCD ID: CUA) (formula: Cu₂).



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 (CCD ID: CUK) (formula: Cu₄S₂).



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 (CCD ID: CA) (formula: Ca).

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

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

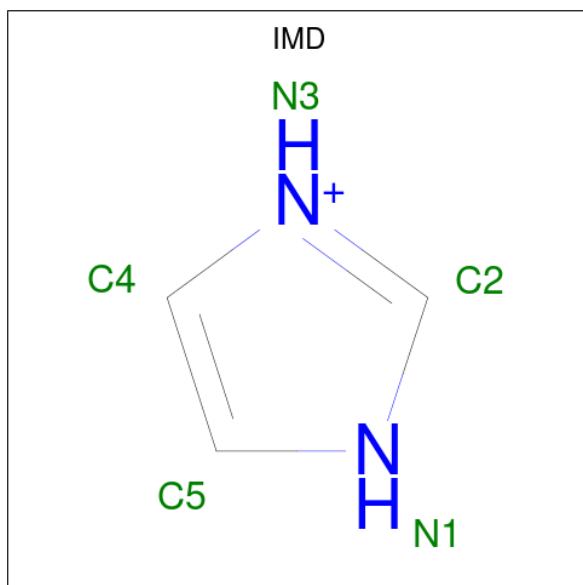
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	K 1	0	0
6	B	1	Total 1	K 1	0	0
6	C	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	E	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total K 1 1	0	0
6	G	1	Total K 1 1	0	0
6	H	1	Total K 1 1	0	0

- Molecule 7 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



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

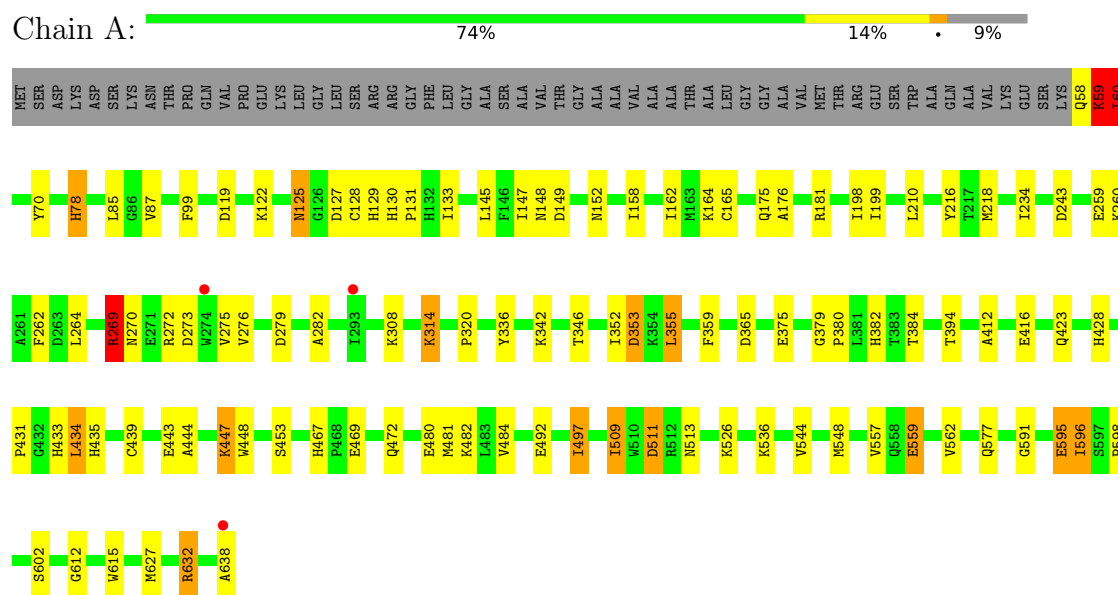
- Molecule 8 is water.

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

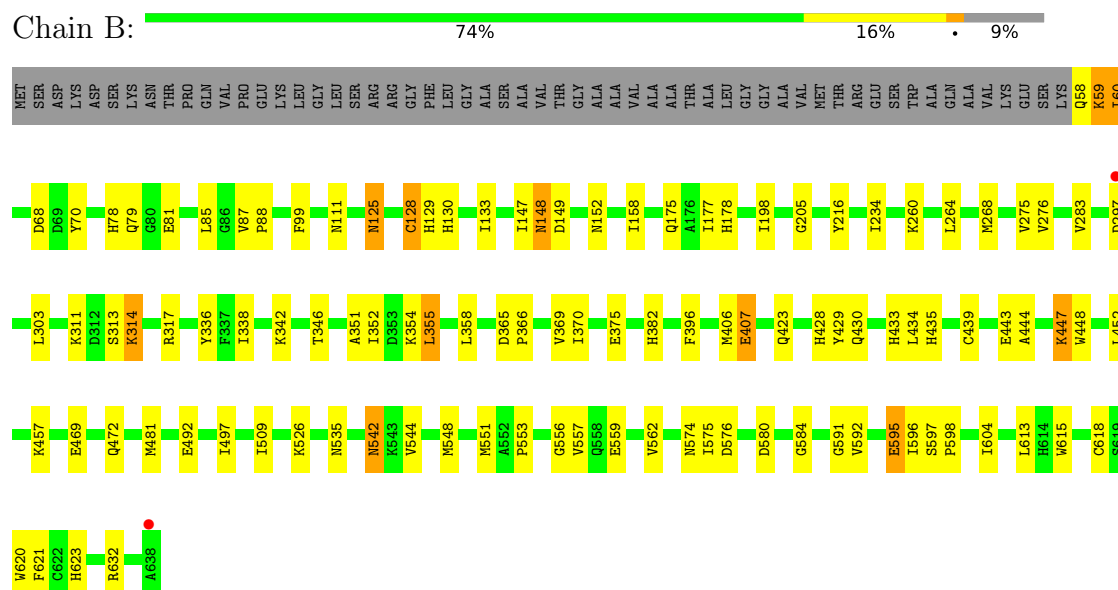
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

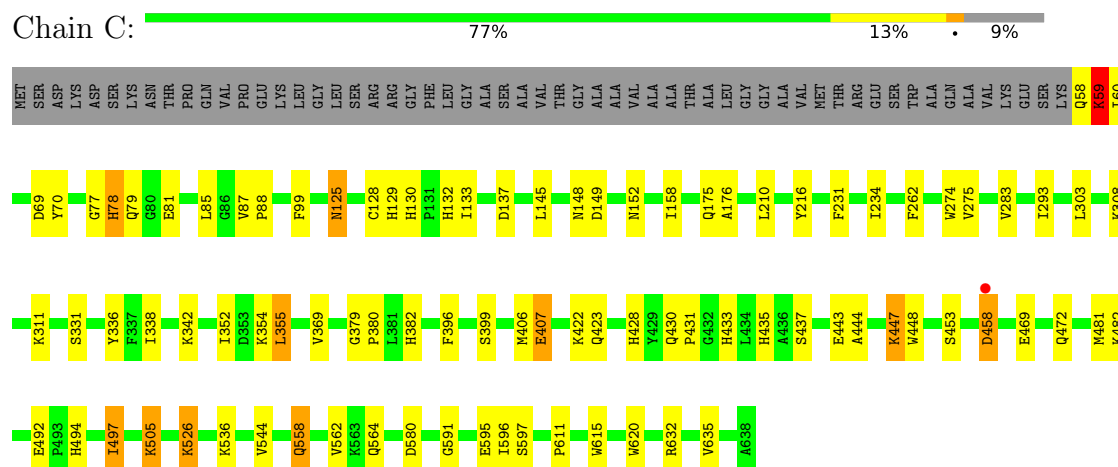
• Molecule 1: Nitrous-oxide reductase



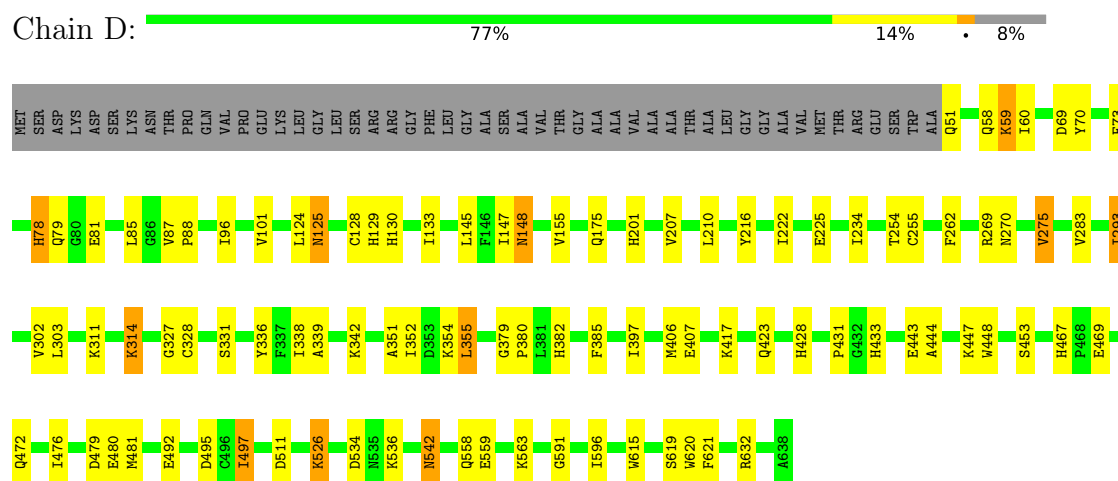
• Molecule 1: Nitrous-oxide reductase



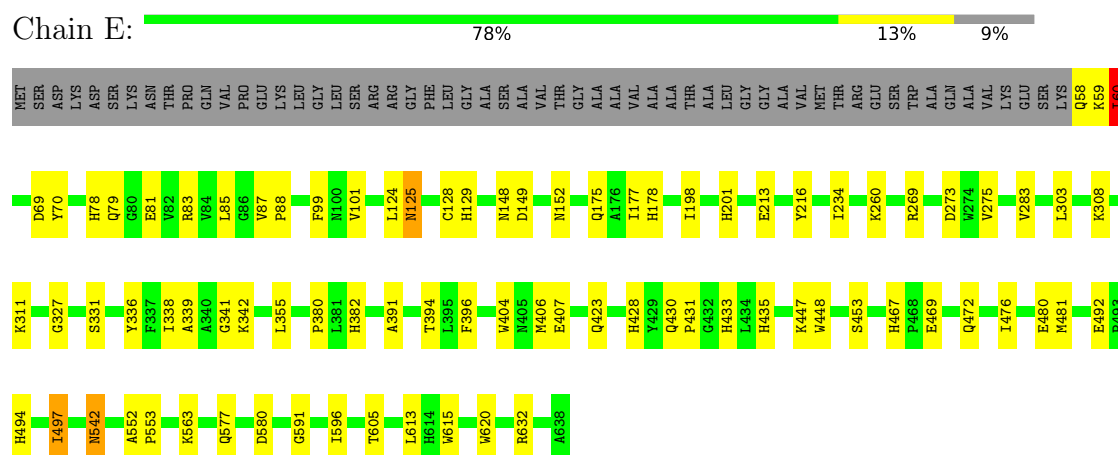
- Molecule 1: Nitrous-oxide reductase



- Molecule 1: Nitrous-oxide reductase

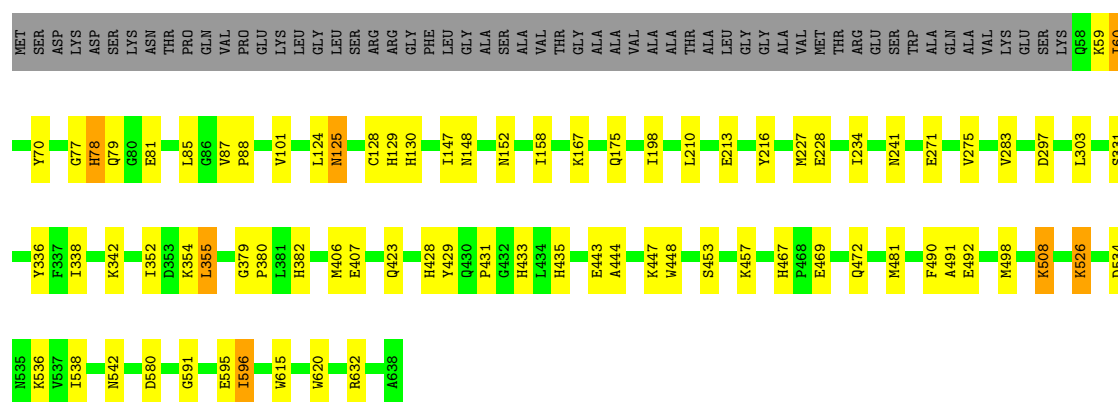


- Molecule 1: Nitrous-oxide reductase



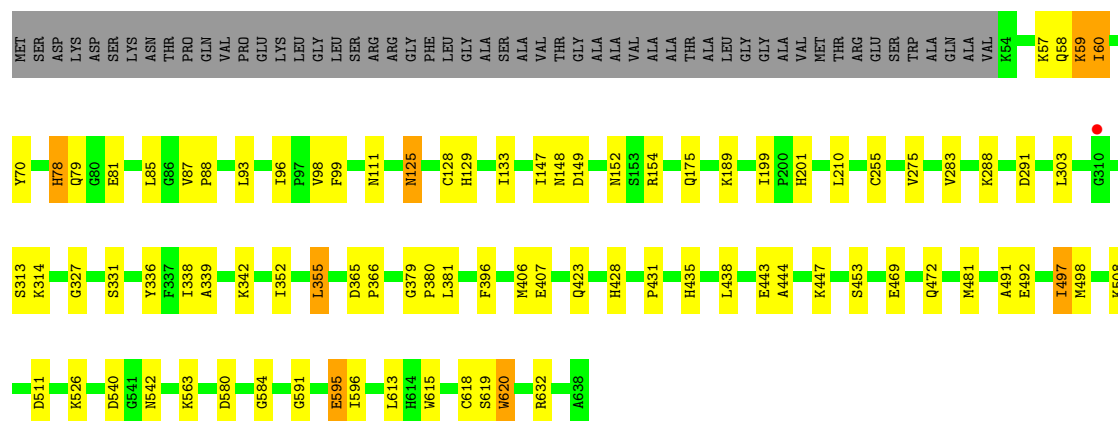
- Molecule 1: Nitrous-oxide reductase

Chain F:  79% 11% 9%



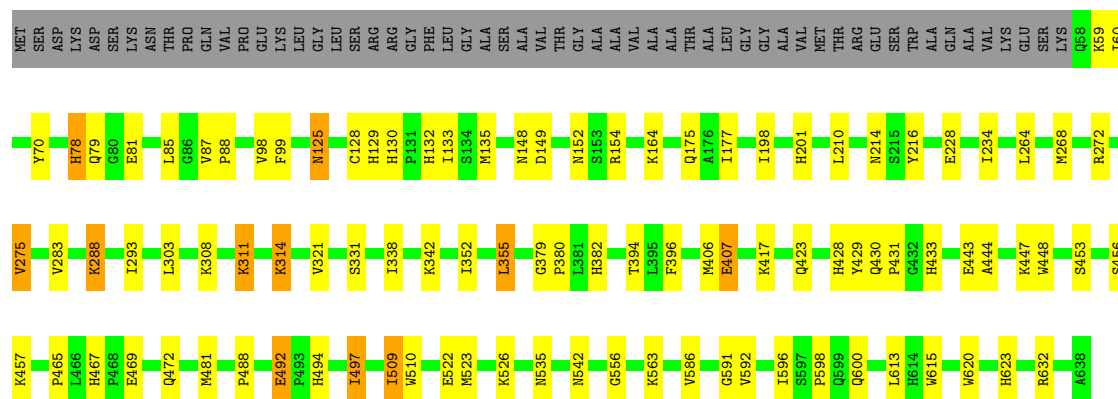
• Molecule 1: Nitrous-oxide reductase

Chain G:  78% 12% 8%



• Molecule 1: Nitrous-oxide reductase

Chain H:  76% 14% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.89Å 106.70Å 131.14Å 111.34° 107.33° 90.74°	Depositor
Resolution (Å)	46.02 – 2.10 46.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.7 (46.02-2.10) 94.7 (46.02-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	39843	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: K, IMD, CUK, CL, CA, CUA

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	0.56	1/4685 (0.0%)	0.83	5/6345 (0.1%)
1	B	0.57	0/4705	0.82	0/6372
1	C	0.66	0/4702	0.86	0/6368
1	D	0.63	1/4748 (0.0%)	0.85	4/6428 (0.1%)
1	E	0.67	2/4687 (0.0%)	0.88	2/6348 (0.0%)
1	F	0.66	1/4705 (0.0%)	0.85	0/6372
1	G	0.64	0/4718	0.87	3/6387 (0.0%)
1	H	0.64	0/4702	0.85	2/6368 (0.0%)
All	All	0.63	5/37652 (0.0%)	0.85	16/50988 (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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	60	ILE	CA-CB	5.74	1.62	1.54
1	E	60	ILE	CA-CB	5.53	1.61	1.54
1	D	275	VAL	CA-CB	5.44	1.60	1.54
1	A	60	ILE	CA-CB	5.25	1.61	1.54
1	E	178	HIS	CA-C	5.01	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ILE	CA-C-N	-6.11	113.39	119.99
1	D	96	ILE	C-N-CA	-6.11	113.39	119.99
1	G	199	ILE	N-CA-C	5.90	114.03	109.19
1	H	492	GLU	CA-C-N	-5.56	114.22	119.89
1	H	492	GLU	C-N-CA	-5.56	114.22	119.89
1	E	273	ASP	N-CA-C	-5.48	104.29	108.78
1	A	365	ASP	CA-C-N	5.36	126.54	119.84
1	A	365	ASP	C-N-CA	5.36	126.54	119.84
1	E	341	GLY	N-CA-C	5.30	120.50	114.67
1	G	96	ILE	CA-C-N	-5.29	114.50	119.85
1	G	96	ILE	C-N-CA	-5.29	114.50	119.85
1	A	199	ILE	N-CA-C	5.27	113.51	109.19
1	D	275	VAL	N-CA-CB	5.22	117.25	110.99
1	A	336	TYR	N-CA-C	5.20	117.89	109.06
1	A	59	LYS	N-CA-C	5.08	121.62	110.80
1	D	534	ASP	N-CA-C	5.05	118.18	110.20

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 [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	4573	0	4441	74	0
1	B	4592	0	4452	86	0
1	C	4590	0	4449	77	0
1	D	4636	0	4505	77	0
1	E	4575	0	4440	71	0
1	F	4593	0	4450	65	0
1	G	4606	0	4478	67	0
1	H	4590	0	4449	77	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	9	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	553	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 8.

All (553) 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:HE3	1.19	1.15
1:C:338:ILE:HD11	1:C:406:MET:HE3	1.25	1.09
1:H:338:ILE:CD1	1:H:406:MET:HE3	1.86	1.05
1:G:331:SER:HB3	1:G:406:MET:HE1	1.38	1.05
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:H:469:GLU:HG3	1:H:492:GLU:HA	1.48	0.96
1:C:458:ASP:HB3	8:C:743:HOH:O	1.66	0.94
1:F:423:GLN:HE22	1:F:481:MET:H	1.12	0.94
1:B:469:GLU:HG3	1:B:492:GLU:HA	1.51	0.93
1:G:283:VAL:HG13	1:G:303:LEU:HD13	1.49	0.93
1:A:125:ASN:HD21	1:B:591:GLY:HA2	1.34	0.92
1:H:283:VAL:HG13	1:H:303:LEU:HD12	1.51	0.90
1:G:288:LYS:HG2	8:G:1278:HOH:O	1.69	0.90
1:A:264:LEU:HD21	1:B:553:PRO:HG2	1.54	0.90
1:E:338:ILE:HD11	1:E:406:MET:HE3	1.54	0.90
1:E:125:ASN:HD21	1:F:591:GLY:HA2	1.38	0.89
1:G:338:ILE:HD11	1:G:406:MET:HE3	1.55	0.88
1:A:269:ARG:HE	1:A:269:ARG:HA	1.39	0.88
1:C:336:TYR:CD2	1:C:406:MET:HE2	2.08	0.88
1:D:352:ILE:HA	1:D:355:LEU:HD22	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:336:TYR:HD2	1:F:406:MET:CE	1.86	0.87
1:B:338:ILE:HD11	1:B:406:MET:HE3	1.57	0.86
1:G:331:SER:CB	1:G:406:MET:HE1	2.05	0.86
1:G:423:GLN:HE22	1:G:481:MET:H	1.23	0.86
1:C:423:GLN:HE22	1:C:481:MET:H	1.19	0.86
1:E:428:HIS:H	1:E:472:GLN:HE22	1.20	0.85
1:G:125:ASN:HD21	1:H:591:GLY:HA2	1.42	0.85
1:H:283:VAL:HG13	1:H:303:LEU:CD1	2.07	0.85
1:D:423:GLN:HE22	1:D:481:MET:H	1.22	0.84
1:C:469:GLU:HG3	1:C:492:GLU:HA	1.60	0.83
1:A:269:ARG:HA	1:A:269:ARG:NE	1.94	0.83
1:C:129:HIS:H	1:C:148:ASN:HD21	1.27	0.82
1:H:129:HIS:H	1:H:148:ASN:HD21	1.28	0.82
1:F:283:VAL:HG13	1:F:303:LEU:HD13	1.60	0.82
1:A:423:GLN:HE22	1:A:481:MET:H	1.27	0.81
1:E:336:TYR:CD2	1:E:406:MET:HE2	2.15	0.81
1:F:129:HIS:H	1:F:148:ASN:HD21	1.29	0.81
1:F:78:HIS:ND1	8:F:2846:HOH:O	2.02	0.80
1:D:133:ILE:HG13	1:D:497:ILE:HD12	1.64	0.79
1:A:259:GLU:HG2	1:A:269:ARG:HB3	1.64	0.79
1:B:423:GLN:HE22	1:B:481:MET:H	1.27	0.79
1:E:125:ASN:ND2	1:F:591:GLY:HA2	1.98	0.79
1:G:563:LYS:HD3	8:G:714:HOH:O	1.81	0.79
1:F:336:TYR:CD2	1:F:406:MET:CE	2.65	0.78
1:C:125:ASN:HD21	1:D:591:GLY:HA2	1.46	0.78
1:G:428:HIS:H	1:G:472:GLN:HE22	1.29	0.78
1:D:428:HIS:H	1:D:472:GLN:HE22	1.30	0.78
1:E:382:HIS:HB3	8:E:1097:HOH:O	1.84	0.77
1:E:336:TYR:HD2	1:E:406:MET:CE	1.98	0.77
1:F:469:GLU:HG3	1:F:492:GLU:HA	1.67	0.76
1:A:577:GLN:CD	8:A:654:HOH:O	2.27	0.76
1:G:469:GLU:HG3	1:G:492:GLU:HA	1.68	0.75
1:F:198:ILE:H	7:F:639:IMD:H2	1.49	0.75
1:E:129:HIS:H	1:E:148:ASN:HD21	1.34	0.75
1:E:269:ARG:HD2	8:E:820:HOH:O	1.86	0.75
1:D:283:VAL:HG13	1:D:303:LEU:HD13	1.68	0.75
1:C:283:VAL:HG13	1:C:303:LEU:CD1	2.17	0.74
1:D:469:GLU:HG3	1:D:492:GLU:HA	1.68	0.74
1:C:428:HIS:H	1:C:472:GLN:HE22	1.36	0.74
1:E:469:GLU:HG3	1:E:492:GLU:HA	1.69	0.74
1:B:129:HIS:H	1:B:148:ASN:HD21	1.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:VAL:HG13	1:E:303:LEU:CD1	2.19	0.73
1:F:336:TYR:CD2	1:F:406:MET:HE2	2.23	0.73
1:E:632:ARG:HD3	8:E:2177:HOH:O	1.87	0.72
1:G:129:HIS:H	1:G:148:ASN:HD21	1.35	0.72
1:D:129:HIS:H	1:D:148:ASN:HD21	1.36	0.72
1:D:336:TYR:HD2	1:D:406:MET:CE	2.02	0.72
1:H:331:SER:HB3	1:H:406:MET:HE1	1.70	0.72
1:C:336:TYR:HD2	1:C:406:MET:HE2	1.52	0.72
1:E:59:LYS:HZ1	1:E:448:TRP:HE1	1.38	0.71
1:E:428:HIS:H	1:E:472:GLN:NE2	1.88	0.71
1:D:632:ARG:HD3	8:D:2130:HOH:O	1.90	0.71
1:D:542:ASN:HB3	8:D:654:HOH:O	1.90	0.71
1:C:382:HIS:CE1	1:C:433:HIS:CE1	2.78	0.71
1:A:469:GLU:HG3	1:A:492:GLU:HA	1.71	0.70
1:E:59:LYS:HE3	1:E:69:ASP:OD2	1.90	0.70
1:E:59:LYS:NZ	1:E:448:TRP:HE1	1.87	0.70
1:E:336:TYR:CD2	1:E:406:MET:CE	2.74	0.70
1:A:352:ILE:HA	1:A:355:LEU:HD22	1.73	0.70
1:B:59:LYS:O	1:B:60:ILE:HG22	1.91	0.70
1:B:542:ASN:C	1:B:542:ASN:HD22	1.99	0.70
1:H:382:HIS:CE1	1:H:433:HIS:CE1	2.79	0.70
1:H:133:ILE:HG13	1:H:497:ILE:HD12	1.73	0.69
1:F:352:ILE:HA	1:F:355:LEU:HD22	1.73	0.69
1:H:509:ILE:HG22	1:H:598:PRO:HB2	1.75	0.68
1:G:336:TYR:HD2	1:G:406:MET:HE2	1.58	0.68
1:D:336:TYR:CD2	1:D:406:MET:HE2	2.29	0.68
1:C:336:TYR:HD2	1:C:406:MET:CE	2.07	0.68
1:E:433:HIS:HB2	1:E:494:HIS:O	1.94	0.68
1:B:428:HIS:H	1:B:472:GLN:HE22	1.40	0.68
1:H:314:LYS:CE	8:H:762:HOH:O	2.42	0.68
1:C:338:ILE:CD1	1:C:406:MET:HE3	2.13	0.68
1:A:125:ASN:ND2	1:B:591:GLY:HA2	2.07	0.68
1:D:338:ILE:HD11	1:D:406:MET:HE3	1.76	0.68
1:D:59:LYS:HZ1	1:D:448:TRP:HE1	1.43	0.67
1:H:314:LYS:HE3	8:H:762:HOH:O	1.94	0.67
1:E:613:LEU:HD11	1:E:632:ARG:HG2	1.75	0.67
1:G:615:TRP:CH2	7:H:639:IMD:H4	2.29	0.67
1:B:70:TYR:HB2	1:B:87:VAL:HB	1.77	0.66
1:E:428:HIS:N	1:E:472:GLN:HE22	1.94	0.66
1:C:133:ILE:HG13	1:C:497:ILE:HD12	1.77	0.66
1:C:338:ILE:HD11	1:C:406:MET:CE	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:VAL:HG13	1:B:303:LEU:HD13	1.77	0.65
1:H:275:VAL:HG13	1:H:321:VAL:HG21	1.78	0.65
1:C:128:CYS:HB3	1:C:148:ASN:O	1.97	0.65
1:H:613:LEU:HD11	1:H:632:ARG:HB3	1.77	0.65
1:C:262:PHE:HB2	1:D:632:ARG:HD2	1.79	0.65
1:E:59:LYS:HE2	1:E:88:PRO:HG3	1.79	0.65
1:G:591:GLY:HA2	1:H:125:ASN:HD21	1.61	0.64
1:C:352:ILE:HA	1:C:355:LEU:HD22	1.79	0.64
1:D:336:TYR:CD2	1:D:406:MET:CE	2.80	0.64
1:F:382:HIS:CE1	1:F:433:HIS:CE1	2.86	0.64
1:H:59:LYS:HE2	1:H:88:PRO:HG3	1.80	0.64
1:A:627:MET:HE1	1:B:178:HIS:CE1	2.33	0.64
1:F:428:HIS:H	1:F:472:GLN:HE22	1.46	0.64
1:F:129:HIS:H	1:F:148:ASN:ND2	1.97	0.63
1:A:544:VAL:HG21	1:A:562:VAL:HG12	1.79	0.63
1:C:331:SER:HB3	1:C:406:MET:HE1	1.79	0.63
1:D:51:GLN:HA	8:D:1483:HOH:O	1.98	0.62
1:D:133:ILE:HG13	1:D:497:ILE:CD1	2.28	0.62
1:E:615:TRP:H	1:F:175:GLN:HE22	1.47	0.62
1:E:70:TYR:HB2	1:E:87:VAL:HB	1.81	0.62
1:B:429:TYR:CD1	1:B:457:LYS:HD2	2.34	0.62
1:C:133:ILE:HG13	1:C:497:ILE:CD1	2.30	0.62
1:C:336:TYR:CD2	1:C:406:MET:CE	2.81	0.62
1:D:431:PRO:HA	1:D:453:SER:HA	1.81	0.62
1:B:469:GLU:CG	1:B:492:GLU:HA	2.28	0.62
1:D:480:GLU:HG3	8:D:1442:HOH:O	2.00	0.62
1:F:338:ILE:HD11	1:F:406:MET:HE3	1.82	0.62
1:B:79:GLN:HE22	1:B:81:GLU:CG	2.13	0.61
1:B:79:GLN:HE22	1:B:81:GLU:HG2	1.64	0.61
1:G:336:TYR:CD2	1:G:406:MET:HE2	2.34	0.61
1:H:59:LYS:NZ	1:H:448:TRP:HE1	1.98	0.61
1:H:128:CYS:HB3	1:H:148:ASN:O	2.00	0.61
1:E:129:HIS:H	1:E:148:ASN:ND2	1.98	0.61
1:A:394:THR:HG23	1:A:434:LEU:HD13	1.83	0.61
1:C:591:GLY:HA2	1:D:125:ASN:HD21	1.66	0.61
1:C:615:TRP:H	1:D:175:GLN:HE22	1.47	0.61
1:H:308:LYS:O	1:H:311:LYS:HD2	2.00	0.60
1:D:293:ILE:HG22	1:D:302:VAL:HB	1.82	0.60
7:H:639:IMD:H5	8:H:688:HOH:O	2.02	0.60
1:E:591:GLY:HA2	1:F:125:ASN:HD21	1.67	0.60
1:F:271[B]:GLU:OE1	8:F:2876:HOH:O	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:595:GLU:HG2	1:G:596:ILE:N	2.17	0.60
1:A:129:HIS:H	1:A:148:ASN:HD21	1.47	0.59
1:A:198:ILE:HD13	1:A:260:LYS:HE3	1.83	0.59
1:G:508:LYS:HE3	8:H:1007:HOH:O	2.02	0.59
1:C:125:ASN:ND2	1:D:591:GLY:HA2	2.16	0.59
1:F:198:ILE:H	7:F:639:IMD:C2	2.15	0.59
1:B:317:ARG:HG3	1:B:358:LEU:HG	1.84	0.59
1:A:577:GLN:HE21	1:A:577:GLN:HA	1.67	0.59
1:C:407:GLU:HG2	1:H:563:LYS:HD2	1.83	0.59
1:G:59:LYS:HE3	1:G:88:PRO:HG3	1.85	0.58
1:B:407:GLU:HG3	8:B:2163:HOH:O	2.01	0.58
1:A:428:HIS:H	1:A:472:GLN:HE22	1.52	0.58
1:E:198:ILE:H	7:E:640:IMD:HN1	1.50	0.58
1:E:336:TYR:HD2	1:E:406:MET:HE2	1.60	0.58
1:D:79:GLN:HE22	1:D:81:GLU:CG	2.17	0.58
1:G:435:HIS:CE1	1:G:497:ILE:HG22	2.39	0.58
1:F:77:GLY:HA2	1:F:128:CYS:O	2.04	0.58
1:H:129:HIS:N	1:H:148:ASN:HD21	2.01	0.58
1:C:129:HIS:H	1:C:148:ASN:ND2	1.98	0.58
1:G:336:TYR:HD2	1:G:406:MET:CE	2.16	0.57
1:D:129:HIS:H	1:D:148:ASN:ND2	2.02	0.57
1:G:59:LYS:O	1:G:60:ILE:HG23	2.05	0.57
1:E:382:HIS:CE1	1:E:433:HIS:CE1	2.93	0.57
1:B:133:ILE:HG13	1:B:497:ILE:HD12	1.85	0.57
1:H:535:ASN:OD1	1:H:556:GLY:HA3	2.04	0.57
1:C:428:HIS:H	1:C:472:GLN:NE2	2.02	0.57
1:C:137:ASP:HB3	8:C:1790:HOH:O	2.03	0.57
1:C:632:ARG:HD3	8:C:2156:HOH:O	2.05	0.57
1:H:308:LYS:O	1:H:311:LYS:CD	2.53	0.57
1:H:129:HIS:H	1:H:148:ASN:ND2	1.99	0.56
1:F:78:HIS:CE1	8:F:2846:HOH:O	2.50	0.56
1:H:79:GLN:HE22	1:H:81:GLU:CG	2.18	0.56
1:D:59:LYS:CE	1:D:88:PRO:HG3	2.35	0.56
1:D:70:TYR:HB2	1:D:87:VAL:HB	1.88	0.56
1:E:447:LYS:HD3	8:E:2352:HOH:O	2.04	0.56
1:E:447:LYS:HE2	8:E:1948:HOH:O	2.05	0.56
1:C:615:TRP:CH2	7:D:639:IMD:H2	2.40	0.55
1:G:615:TRP:CZ2	7:H:639:IMD:H4	2.41	0.55
1:B:352:ILE:HA	1:B:355:LEU:HD22	1.87	0.55
1:B:264:LEU:HG	1:B:268:MET:HE2	1.89	0.55
1:F:70:TYR:HB2	1:F:87:VAL:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HD13	1:A:484:VAL:HB	1.88	0.55
1:A:70:TYR:HB2	1:A:87:VAL:HB	1.88	0.55
1:F:632:ARG:HD3	8:F:1451:HOH:O	2.07	0.55
1:A:509:ILE:HG22	1:A:598:PRO:HB2	1.89	0.55
1:B:125:ASN:ND2	1:B:152:ASN:HD21	2.03	0.55
1:E:283:VAL:HG13	1:E:303:LEU:HD13	1.88	0.55
1:A:615:TRP:H	1:B:175:GLN:HE22	1.55	0.55
1:G:632:ARG:HD3	8:G:2045:HOH:O	2.07	0.55
1:C:632:ARG:HD2	1:D:262:PHE:HB2	1.89	0.54
1:C:129:HIS:N	1:C:148:ASN:HD21	2.01	0.54
1:C:431:PRO:HA	1:C:453:SER:HA	1.88	0.54
1:G:619:SER:O	1:H:78:HIS:CE1	2.61	0.54
1:D:73:PHE:HB2	1:D:497:ILE:HG13	1.90	0.54
1:H:431:PRO:HA	1:H:453:SER:HA	1.90	0.54
1:H:396:PHE:CE1	1:H:430:GLN:HB3	2.43	0.54
1:A:272:ARG:HD2	8:A:968:HOH:O	2.07	0.54
1:F:59:LYS:HE2	1:F:448:TRP:HZ2	1.73	0.54
1:F:125:ASN:ND2	1:F:152:ASN:HD21	2.06	0.54
1:G:70:TYR:HB2	1:G:87:VAL:HB	1.90	0.54
1:G:431:PRO:HA	1:G:453:SER:HA	1.90	0.54
1:H:132:HIS:HA	1:H:497:ILE:HD13	1.90	0.54
1:H:314:LYS:HD3	8:H:2281:HOH:O	2.07	0.54
1:H:428:HIS:H	1:H:472:GLN:HE22	1.56	0.54
1:A:262:PHE:HB2	1:B:632:ARG:HD2	1.90	0.54
1:A:591:GLY:HA2	1:B:125:ASN:HD21	1.72	0.54
1:C:70:TYR:HB2	1:C:87:VAL:HB	1.88	0.54
1:F:128:CYS:HB2	1:F:147:ILE:HG12	1.90	0.54
1:E:396:PHE:CE1	1:E:430:GLN:HB3	2.43	0.53
1:F:428:HIS:H	1:F:472:GLN:NE2	2.06	0.53
1:A:382:HIS:CE1	1:A:433:HIS:CE1	2.97	0.53
1:C:526:LYS:HB2	1:C:526:LYS:NZ	2.24	0.53
1:E:101:VAL:HG21	1:E:124:LEU:HD22	1.90	0.53
1:F:443:GLU:O	1:F:444:ALA:C	2.51	0.53
1:G:79:GLN:HE22	1:G:81:GLU:CG	2.20	0.53
1:G:469:GLU:CG	1:G:492:GLU:HA	2.39	0.53
1:G:125:ASN:ND2	1:H:591:GLY:HA2	2.18	0.53
1:H:429:TYR:CD2	1:H:457:LYS:HD2	2.43	0.53
1:B:497:ILE:HG21	8:B:2451:HOH:O	2.09	0.53
1:D:331:SER:CB	1:D:406:MET:HE1	2.39	0.53
1:G:435:HIS:HD2	1:G:498:MET:HE3	1.73	0.53
1:F:331:SER:HB3	1:F:406:MET:HE1	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ILE:CG1	1:D:497:ILE:HD12	2.36	0.52
1:E:125:ASN:ND2	1:E:152:ASN:HD21	2.07	0.52
1:D:526:LYS:HD3	8:D:1185:HOH:O	2.10	0.52
1:E:129:HIS:N	1:E:148:ASN:HD21	2.03	0.52
1:A:269:ARG:NE	1:A:269:ARG:CA	2.66	0.52
1:D:51:GLN:HG3	1:E:605:THR:CG2	2.40	0.52
1:F:354:LYS:NZ	8:F:777:HOH:O	2.42	0.52
1:G:128:CYS:HB2	1:G:147:ILE:HG12	1.90	0.52
1:D:78:HIS:ND1	8:D:2779:HOH:O	2.11	0.52
1:A:480:GLU:OE1	1:F:526:LYS:HE2	2.10	0.52
1:D:130:HIS:H	1:D:148:ASN:ND2	2.08	0.52
1:H:586:VAL:HA	1:H:592:VAL:O	2.09	0.52
1:C:125:ASN:ND2	1:C:152:ASN:HD21	2.08	0.51
1:D:269:ARG:NH1	1:D:270:ASN:OD1	2.43	0.51
1:E:591:GLY:HA2	1:F:125:ASN:ND2	2.25	0.51
1:G:615:TRP:H	1:H:175:GLN:HE22	1.58	0.51
1:B:595:GLU:HB2	1:B:620:TRP:CZ3	2.46	0.51
1:B:125:ASN:HD21	1:B:152:ASN:HD21	1.57	0.51
1:F:125:ASN:HD21	1:F:152:ASN:HD21	1.58	0.51
1:A:210:LEU:O	1:A:260:LYS:HE2	2.10	0.51
1:B:428:HIS:HB3	1:B:429:TYR:CE1	2.45	0.51
1:A:175:GLN:HE22	1:B:615:TRP:H	1.57	0.51
1:D:51:GLN:HG3	1:E:605:THR:HG21	1.93	0.51
1:C:331:SER:CB	1:C:406:MET:HE1	2.40	0.51
1:B:382[A]:HIS:CE1	1:B:433:HIS:CE1	2.99	0.51
1:E:59:LYS:O	1:E:60:ILE:HG23	2.11	0.51
1:A:282:ALA:HB1	1:A:314:LYS:HD2	1.92	0.51
1:C:59:LYS:HE3	1:C:69:ASP:OD2	2.10	0.51
8:D:715:HOH:O	7:E:639:IMD:H5	2.10	0.51
1:A:133:ILE:HG13	1:A:497:ILE:HD13	1.93	0.51
1:H:59:LYS:HZ3	1:H:448:TRP:HE1	1.56	0.51
1:A:99:PHE:CE2	1:A:149:ASP:HB2	2.46	0.50
1:A:130:HIS:H	1:A:148:ASN:ND2	2.09	0.50
1:G:148:ASN:HD22	1:G:148:ASN:H	1.58	0.50
1:H:198:ILE:H	7:H:639:IMD:HN3	1.59	0.50
1:H:214:ASN:ND2	8:H:751:HOH:O	2.45	0.50
1:A:577:GLN:HA	1:A:577:GLN:NE2	2.27	0.50
1:D:476:ILE:HG22	1:D:481:MET:HG2	1.94	0.50
1:A:467:HIS:HB2	1:B:580:ASP:OD1	2.12	0.50
1:B:428:HIS:H	1:B:472:GLN:NE2	2.07	0.50
1:B:452:LEU:N	1:B:452:LEU:HD12	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ASN:ND2	1:G:152:ASN:HD21	2.09	0.50
1:G:331:SER:HB3	1:G:406:MET:CE	2.27	0.50
1:C:536:LYS:HE2	8:C:1127:HOH:O	2.10	0.50
1:C:175:GLN:HE22	1:D:615:TRP:H	1.59	0.50
1:E:175:GLN:HE22	1:F:615:TRP:H	1.60	0.50
1:G:352:ILE:HA	1:G:355:LEU:HD22	1.93	0.50
1:B:125:ASN:HD22	1:B:125:ASN:H	1.59	0.50
1:C:379:GLY:N	1:C:380:PRO:HD3	2.26	0.50
1:D:331:SER:HB3	1:D:406:MET:HE1	1.94	0.50
1:F:336:TYR:HD2	1:F:406:MET:HE1	1.73	0.50
1:C:433:HIS:HB2	1:C:494:HIS:O	2.12	0.50
1:H:125:ASN:ND2	1:H:152:ASN:HD21	2.10	0.50
1:A:412:ALA:HA	1:A:416:GLU:O	2.12	0.49
1:B:351:ALA:HB3	1:B:354:LYS:HG3	1.93	0.49
1:E:336:TYR:HD2	1:E:406:MET:HE1	1.74	0.49
1:D:559:GLU:HA	1:D:632:ARG:O	2.12	0.49
1:G:540:ASP:HB3	8:G:699:HOH:O	2.12	0.49
1:G:591:GLY:HA2	1:H:125:ASN:ND2	2.27	0.49
1:C:216:TYR:CD1	1:C:234:ILE:HG23	2.47	0.49
8:G:1326:HOH:O	1:H:465:PRO:HD2	2.13	0.49
1:A:443:GLU:O	1:A:444:ALA:C	2.55	0.49
1:E:331:SER:HB3	1:E:406:MET:HE1	1.94	0.49
1:G:365:ASP:OD1	1:G:366:PRO:HD2	2.12	0.49
1:A:58:GLN:HE22	1:A:447:LYS:HG2	1.78	0.49
1:A:125:ASN:ND2	1:A:152:ASN:HD21	2.11	0.49
7:E:640:IMD:H2	1:F:615:TRP:CZ2	2.47	0.49
1:H:379:GLY:N	1:H:380:PRO:HD3	2.27	0.49
1:C:435:HIS:CE1	1:C:497:ILE:HG22	2.48	0.49
1:D:59:LYS:HE2	1:D:88:PRO:HG3	1.94	0.49
1:D:201:HIS:HE1	1:D:216:TYR:O	1.95	0.49
1:F:534:ASP:HB3	1:F:536:LYS:HD2	1.94	0.49
1:G:129:HIS:H	1:G:148:ASN:ND2	2.07	0.49
1:E:58:GLN:N	8:E:1461:HOH:O	2.46	0.49
1:D:379:GLY:N	1:D:380:PRO:HD3	2.27	0.48
1:C:79:GLN:HE22	1:C:81:GLU:CG	2.25	0.48
1:E:338:ILE:HD11	1:E:406:MET:CE	2.34	0.48
1:B:79:GLN:NE2	1:B:81:GLU:HG2	2.29	0.48
1:E:580:ASP:OD1	1:F:467:HIS:HB2	2.14	0.48
1:G:175:GLN:HE22	1:H:615:TRP:H	1.59	0.48
1:B:542:ASN:C	1:B:542:ASN:ND2	2.71	0.48
1:D:428:HIS:H	1:D:472:GLN:NE2	2.04	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:580:ASP:OD1	1:H:467:HIS:HB2	2.13	0.48
1:E:99:PHE:CE2	1:E:149:ASP:HB2	2.49	0.48
1:H:125:ASN:HD21	1:H:152:ASN:HD21	1.62	0.48
1:F:336:TYR:CE2	1:F:406:MET:HE2	2.49	0.48
1:H:216:TYR:CD1	1:H:234:ILE:HG23	2.49	0.48
1:A:129:HIS:H	1:A:148:ASN:ND2	2.10	0.47
1:C:443:GLU:O	1:C:444:ALA:C	2.57	0.47
1:F:429:TYR:CD1	1:F:457:LYS:HD2	2.49	0.47
1:A:125:ASN:HD21	1:A:152:ASN:HD21	1.61	0.47
1:F:447:LYS:HE2	8:F:2850:HOH:O	2.14	0.47
1:F:379:GLY:N	1:F:380:PRO:HD3	2.29	0.47
1:H:382:HIS:CD2	1:H:433:HIS:HA	2.50	0.47
1:B:338:ILE:HD11	1:B:406:MET:CE	2.37	0.47
1:B:148:ASN:H	1:B:148:ASN:HD22	1.63	0.47
1:G:78:HIS:ND1	8:G:2902:HOH:O	2.08	0.47
1:B:336:TYR:CD2	1:B:406:MET:CE	2.98	0.47
1:C:492:GLU:OE2	1:D:621:PHE:HB2	2.15	0.47
1:D:314:LYS:HB3	1:D:314:LYS:HE3	1.48	0.47
1:E:467:HIS:HB2	1:F:580:ASP:OD1	2.14	0.47
1:A:131:PRO:O	1:A:497:ILE:HG12	2.15	0.47
1:B:59:LYS:NZ	1:B:448:TRP:HE1	2.12	0.47
1:C:399[B]:SER:O	1:C:399[B]:SER:OG	2.31	0.47
1:E:327:GLY:O	1:E:339:ALA:HA	2.15	0.47
1:A:119:ASP:O	1:A:122:LYS:HG2	2.16	0.46
1:H:428:HIS:H	1:H:472:GLN:NE2	2.13	0.46
1:D:148:ASN:H	1:D:148:ASN:HD22	1.64	0.46
1:G:99:PHE:CE2	1:G:149:ASP:HB2	2.50	0.46
1:A:59:LYS:NZ	1:A:448:TRP:HE1	2.12	0.46
1:B:111:ASN:ND2	8:B:2638:HOH:O	2.48	0.46
1:C:99:PHE:CE2	1:C:149:ASP:HB2	2.50	0.46
1:G:125:ASN:HD22	1:G:125:ASN:H	1.63	0.46
1:G:428:HIS:H	1:G:472:GLN:NE2	2.05	0.46
1:G:613:LEU:HD11	1:G:632:ARG:HG2	1.97	0.46
1:D:59:LYS:O	8:D:2707:HOH:O	2.21	0.46
1:D:479:ASP:CB	8:D:1442:HOH:O	2.63	0.46
1:B:128:CYS:HB3	1:B:148:ASN:O	2.14	0.46
1:D:145:LEU:CD1	1:D:497:ILE:HD11	2.45	0.46
1:E:216:TYR:CD1	1:E:234:ILE:HG23	2.51	0.46
1:A:162:ILE:HD12	1:A:164:LYS:HB2	1.97	0.46
1:A:379:GLY:N	1:A:380:PRO:HD3	2.30	0.46
1:C:615:TRP:CZ3	7:D:639:IMD:H2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:GLY:HA2	1:C:128:CYS:O	2.15	0.46
1:D:59:LYS:HE3	1:D:88:PRO:HG3	1.97	0.46
1:B:382[B]:HIS:HD2	1:B:434:LEU:HD23	1.80	0.45
1:D:443:GLU:O	1:D:444:ALA:C	2.58	0.45
1:G:59:LYS:HB3	1:G:60:ILE:H	1.32	0.45
1:B:336:TYR:HD2	1:B:406:MET:CE	2.29	0.45
1:C:137:ASP:CB	8:C:1790:HOH:O	2.63	0.45
1:E:336:TYR:CE2	1:E:406:MET:HE2	2.51	0.45
1:A:145:LEU:C	1:A:145:LEU:HD23	2.42	0.45
1:C:423:GLN:HE22	1:C:481:MET:N	2.00	0.45
1:G:443:GLU:O	1:G:444:ALA:C	2.59	0.45
1:G:595:GLU:HB2	1:G:620:TRP:CZ3	2.51	0.45
1:C:580:ASP:OD1	1:D:467:HIS:HB2	2.15	0.45
1:F:490:PHE:CE2	1:F:491:ALA:HB2	2.51	0.45
1:B:346:THR:HG22	1:B:375:GLU:HA	1.99	0.45
1:D:128:CYS:HB2	1:D:147:ILE:HG12	1.99	0.45
1:A:492:GLU:OE2	1:B:621:PHE:HB2	2.17	0.45
1:A:591:GLY:HA2	1:B:125:ASN:ND2	2.31	0.45
1:B:314:LYS:O	1:B:314:LYS:HG2	2.17	0.45
1:E:431:PRO:HA	1:E:453:SER:HA	1.97	0.45
1:F:59:LYS:HE2	1:F:448:TRP:CZ2	2.51	0.45
1:H:443:GLU:O	1:H:444:ALA:C	2.58	0.45
1:F:79:GLN:HE22	1:F:81:GLU:CG	2.30	0.45
1:B:574:ASN:HD22	1:B:597:SER:C	2.25	0.45
1:C:148:ASN:HD22	1:C:148:ASN:H	1.65	0.45
1:D:101:VAL:HG21	1:D:124:LEU:HD22	1.99	0.45
1:H:407:GLU:OE1	8:H:2968:HOH:O	2.21	0.45
1:E:79:GLN:NE2	1:E:83:ARG:HH21	2.14	0.45
1:H:149:ASP:HB3	1:H:154:ARG:HB2	1.99	0.45
1:A:78:HIS:HA	1:A:127:ASP:HA	1.99	0.44
1:A:273:ASP:O	1:A:320:PRO:HA	2.17	0.44
1:A:435:HIS:CE1	1:A:439:CYS:SG	3.10	0.44
1:D:59:LYS:HE3	1:D:69:ASP:OD2	2.17	0.44
1:D:128:CYS:HB3	1:D:148:ASN:O	2.17	0.44
1:D:382:HIS:CE1	1:D:433:HIS:NE2	2.85	0.44
1:F:129:HIS:N	1:F:148:ASN:HD21	2.07	0.44
1:B:535:ASN:OD1	1:B:556:GLY:HA3	2.17	0.44
1:C:494:HIS:HE1	8:D:1439:HOH:O	1.99	0.44
1:C:611:PRO:HA	1:C:635:VAL:HB	1.99	0.44
1:D:563:LYS:HE3	1:D:563:LYS:HB2	1.84	0.44
1:G:201:HIS:HD2	8:G:984:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:NH2	8:A:1918:HOH:O	2.47	0.44
1:D:336:TYR:CE2	1:D:406:MET:HE2	2.52	0.44
1:F:331:SER:CB	1:F:406:MET:HE1	2.47	0.44
1:E:99:PHE:CZ	1:E:149:ASP:HB2	2.52	0.44
1:E:128:CYS:HB3	1:E:148:ASN:O	2.18	0.44
1:H:70:TYR:HB2	1:H:87:VAL:HB	1.99	0.44
1:B:58:GLN:HE22	1:B:447:LYS:CG	2.30	0.44
1:B:336:TYR:CD2	1:B:406:MET:HE2	2.52	0.44
1:B:435:HIS:CE1	1:B:439:CYS:SG	3.11	0.44
1:E:125:ASN:HD21	1:E:152:ASN:HD21	1.66	0.44
1:A:128:CYS:HB2	1:A:147:ILE:HG12	2.00	0.44
1:C:125:ASN:HD21	1:C:152:ASN:HD21	1.64	0.44
1:G:584:GLY:O	1:G:618:CYS:HA	2.18	0.44
1:H:563:LYS:HE2	8:H:755:HOH:O	2.18	0.44
1:E:563:LYS:HB2	1:E:563:LYS:HE3	1.67	0.44
1:B:365:ASP:OD1	1:B:366:PRO:HD2	2.18	0.43
1:C:396:PHE:CE1	1:C:430:GLN:HB3	2.53	0.43
1:F:241:ASN:ND2	5:F:704:CL:CL	2.88	0.43
1:H:99:PHE:CE2	1:H:149:ASP:HB2	2.53	0.43
1:C:231:PHE:CE1	1:C:283:VAL:HG11	2.53	0.43
1:E:577:GLN:HE21	1:E:577:GLN:HB3	1.65	0.43
1:F:101:VAL:HG21	1:F:124:LEU:HD22	1.99	0.43
1:F:148:ASN:H	1:F:148:ASN:HD22	1.65	0.43
1:F:431:PRO:HA	1:F:453:SER:HA	1.98	0.43
1:H:135:MET:HE3	1:H:135:MET:HB2	1.94	0.43
1:H:352:ILE:HA	1:H:355:LEU:HD22	1.99	0.43
1:H:542:ASN:HB3	8:H:1267:HOH:O	2.19	0.43
1:D:536:LYS:HG2	8:D:2767:HOH:O	2.17	0.43
1:E:469:GLU:CG	1:E:492:GLU:HA	2.44	0.43
1:F:130:HIS:H	1:F:148:ASN:ND2	2.17	0.43
1:G:149:ASP:HB3	1:G:154:ARG:HB2	2.00	0.43
1:H:456:SER:O	1:H:457:LYS:C	2.60	0.43
1:A:638:ALA:HA	8:A:1042:HOH:O	2.17	0.43
1:B:59:LYS:HA	8:B:2512:HOH:O	2.18	0.43
1:C:130:HIS:H	1:C:148:ASN:ND2	2.16	0.43
1:F:595:GLU:HG2	1:F:596:ILE:N	2.33	0.43
1:B:366:PRO:O	1:B:369:VAL:HG22	2.18	0.43
1:F:59:LYS:HE3	1:F:88:PRO:HG3	2.01	0.43
1:G:125:ASN:HD21	1:G:152:ASN:HD21	1.65	0.43
1:A:181:ARG:HD2	1:A:243:ASP:CG	2.43	0.43
1:C:59:LYS:NZ	1:C:448:TRP:HE1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:THR:HG23	1:D:328:CYS:HB2	2.01	0.43
1:G:79:GLN:HE22	1:G:81:GLU:HG2	1.83	0.43
1:H:264:LEU:HG	1:H:268:MET:HE2	2.01	0.43
1:A:158:ILE:HA	1:A:165:CYS:HA	2.00	0.43
1:A:379:GLY:H	1:A:380:PRO:HD3	1.83	0.43
1:A:548:MET:HE2	1:A:557:VAL:HB	2.00	0.43
1:B:613:LEU:HD11	1:B:632:ARG:HB3	2.00	0.43
1:G:111:ASN:ND2	8:G:691:HOH:O	2.52	0.43
1:C:78:HIS:CE1	1:D:619:SER:O	2.72	0.43
1:E:494:HIS:HE1	8:F:1431:HOH:O	2.01	0.43
1:F:382:HIS:CD2	1:F:433:HIS:HA	2.54	0.43
1:G:291:ASP:HB3	8:G:2572:HOH:O	2.17	0.43
1:B:58:GLN:HE22	1:B:447:LYS:HG3	1.83	0.43
1:C:145:LEU:HD22	1:C:158:ILE:HD12	2.01	0.43
1:B:130:HIS:H	1:B:148:ASN:ND2	2.16	0.42
1:B:509:ILE:HG22	1:B:598:PRO:HB2	2.01	0.42
1:F:167:LYS:HB2	1:F:227:MET:HG3	2.01	0.42
1:B:435:HIS:CE1	1:B:497:ILE:HG22	2.53	0.42
1:C:125:ASN:HD22	1:C:125:ASN:H	1.66	0.42
1:E:380:PRO:HA	1:E:394:THR:O	2.19	0.42
1:F:198:ILE:N	7:F:639:IMD:H2	2.26	0.42
1:F:407:GLU:OE1	8:F:2856:HOH:O	2.21	0.42
1:G:327:GLY:O	1:G:339:ALA:HA	2.19	0.42
1:H:148:ASN:HB2	1:H:177:ILE:HG22	2.01	0.42
1:A:612:GLY:HA2	1:B:205:GLY:HA2	2.02	0.42
1:G:99:PHE:CZ	1:G:149:ASP:HB2	2.53	0.42
1:H:433:HIS:HB2	1:H:494:HIS:O	2.19	0.42
1:B:128:CYS:HB2	1:B:147:ILE:HD11	2.02	0.42
1:B:129:HIS:H	1:B:148:ASN:ND2	2.10	0.42
1:C:564:GLN:NE2	8:C:680:HOH:O	2.42	0.42
1:E:79:GLN:HE21	1:E:83:ARG:HH21	1.67	0.42
1:E:552:ALA:HA	1:E:553:PRO:HA	1.83	0.42
1:F:216:TYR:CD1	1:F:234:ILE:HG23	2.54	0.42
1:G:79:GLN:HB2	1:G:491:ALA:CB	2.50	0.42
1:A:380:PRO:HA	1:A:394:THR:O	2.19	0.42
1:G:133:ILE:HG13	1:G:497:ILE:CD1	2.49	0.42
1:B:198:ILE:HD13	1:B:260:LYS:HG2	2.01	0.42
1:D:331:SER:HA	1:D:385:PHE:CE2	2.53	0.42
1:F:508:LYS:HE2	8:F:2836:HOH:O	2.20	0.42
1:G:93:LEU:HD23	1:H:488:PRO:HG3	2.02	0.42
1:G:379:GLY:N	1:G:380:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:381:LEU:CD1	1:G:396:PHE:HB2	2.50	0.42
1:G:381:LEU:HD11	1:G:396:PHE:HB2	2.00	0.42
1:B:336:TYR:HD2	1:B:406:MET:HE1	1.84	0.42
1:B:548:MET:HE2	1:B:557:VAL:HB	2.02	0.42
1:C:354:LYS:HD3	1:C:369:VAL:HA	2.00	0.42
1:F:128:CYS:HB3	1:F:148:ASN:O	2.20	0.42
1:A:431:PRO:HA	1:A:453:SER:HA	2.00	0.42
1:H:130:HIS:H	1:H:148:ASN:ND2	2.18	0.42
1:A:577:GLN:HE21	1:A:577:GLN:CA	2.29	0.42
1:C:469:GLU:CG	1:C:492:GLU:HA	2.40	0.42
1:B:314:LYS:HE2	1:B:314:LYS:HB3	1.69	0.42
1:B:595:GLU:HB2	1:B:620:TRP:CH2	2.55	0.42
1:C:58:GLN:HE22	1:C:447:LYS:HG3	1.85	0.42
1:D:433:HIS:ND1	1:D:495:ASP:CG	2.78	0.42
1:D:155:VAL:HG21	1:D:222:ILE:CD1	2.50	0.41
1:E:79:GLN:HE22	1:E:81:GLU:CG	2.32	0.41
1:E:148:ASN:HB2	1:E:177:ILE:HG22	2.01	0.41
1:E:476:ILE:HG22	1:E:481:MET:HG2	2.02	0.41
1:F:59:LYS:HG2	8:F:1420:HOH:O	2.19	0.41
1:D:216:TYR:CD1	1:D:234:ILE:HG23	2.56	0.41
1:E:391:ALA:HB3	1:E:404:TRP:CE2	2.54	0.41
8:E:1197:HOH:O	1:H:288:LYS:HE3	2.18	0.41
1:A:511:ASP:HB3	1:A:513:ASN:OD1	2.20	0.41
1:B:99:PHE:CE2	1:B:149:ASP:HB2	2.55	0.41
1:C:595:GLU:OE2	1:C:597:SER:OG	2.29	0.41
1:B:59:LYS:HE2	1:B:88:PRO:HG3	2.02	0.41
1:B:68:ASP:HB3	1:B:87:VAL:O	2.21	0.41
1:B:148:ASN:HB2	1:B:177:ILE:HG22	2.02	0.41
1:B:443:GLU:O	1:B:444:ALA:C	2.62	0.41
1:B:544:VAL:HG21	1:B:562:VAL:HG12	2.02	0.41
1:B:592:VAL:HG13	1:B:604:ILE:HD13	2.01	0.41
1:D:79:GLN:HE22	1:D:81:GLU:HG2	1.83	0.41
1:H:469:GLU:HG3	1:H:492:GLU:CA	2.36	0.41
1:C:132:HIS:HA	1:C:497:ILE:HD13	2.03	0.41
1:C:422:LYS:HA	1:C:422:LYS:HD3	1.94	0.41
1:H:125:ASN:HD22	1:H:125:ASN:H	1.68	0.41
1:H:510:TRP:CD1	1:H:600:GLN:HB2	2.56	0.41
1:A:78:HIS:CE1	1:A:492:GLU:HB3	2.55	0.41
1:B:59:LYS:HB3	1:B:60:ILE:H	1.57	0.41
1:B:396:PHE:CE1	1:B:430:GLN:HB3	2.55	0.41
8:D:2328:HOH:O	7:E:639:IMD:H4	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:LYS:HD2	8:E:642:HOH:O	2.20	0.41
1:A:218:MET:HG2	1:A:234:ILE:HA	2.01	0.41
1:A:279:ASP:HB2	1:A:359:PHE:CE2	2.56	0.41
1:A:595:GLU:HG2	1:A:596:ILE:N	2.35	0.41
1:B:553:PRO:HG3	1:B:623:HIS:CE1	2.56	0.41
1:D:133:ILE:CD1	1:D:497:ILE:HD12	2.51	0.41
1:D:145:LEU:HD11	1:D:497:ILE:HD11	2.01	0.41
1:H:148:ASN:H	1:H:148:ASN:HD22	1.69	0.41
1:C:591:GLY:HA2	1:D:125:ASN:ND2	2.34	0.41
1:D:351:ALA:HB3	1:D:354:LYS:HG3	2.02	0.41
1:D:382:HIS:NE2	1:D:433:HIS:CD2	2.89	0.41
1:A:423:GLN:HE22	1:A:481:MET:N	2.07	0.41
1:A:536:LYS:CD	8:A:650:HOH:O	2.68	0.41
1:A:559:GLU:OE1	1:A:632:ARG:NH1	2.53	0.41
1:C:544:VAL:HG21	1:C:562:VAL:HG12	2.03	0.41
1:E:435:HIS:CE1	1:E:497:ILE:HA	2.56	0.41
1:G:125:ASN:HD22	1:G:125:ASN:N	2.19	0.41
1:H:509:ILE:HD12	8:H:943:HOH:O	2.19	0.41
1:B:59:LYS:O	1:B:60:ILE:CG2	2.65	0.41
1:C:59:LYS:HE2	1:C:88:PRO:HG3	2.03	0.41
1:C:505:LYS:HE3	1:C:505:LYS:HB3	1.85	0.41
1:C:558:GLN:HE21	1:C:558:GLN:HB3	1.68	0.41
1:G:497:ILE:HB	8:G:675:HOH:O	2.20	0.41
1:B:133:ILE:HG13	1:B:497:ILE:CD1	2.48	0.40
1:B:216:TYR:CD1	1:B:234:ILE:HG23	2.57	0.40
1:E:201:HIS:HD2	8:E:2808:HOH:O	2.04	0.40
1:A:216:TYR:CD1	1:A:234:ILE:HG23	2.56	0.40
1:A:346:THR:HG22	1:A:375:GLU:HA	2.03	0.40
1:A:384:THR:HG22	1:A:434:LEU:HG	2.03	0.40
1:B:584:GLY:O	1:B:618:CYS:HA	2.22	0.40
1:D:327:GLY:O	1:D:339:ALA:HA	2.22	0.40
1:D:469:GLU:CG	1:D:492:GLU:HA	2.46	0.40
1:F:435:HIS:HD2	1:F:498:MET:HE3	1.87	0.40
1:H:447:LYS:HD3	8:H:1866:HOH:O	2.22	0.40
1:H:129:HIS:CE1	1:H:494:HIS:CE1	3.10	0.40
1:H:201:HIS:HE1	1:H:216:TYR:O	2.04	0.40
1:H:272:ARG:NH2	8:H:682:HOH:O	2.42	0.40
1:H:380:PRO:HA	1:H:394:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/638 (91%)	544 (94%)	30 (5%)	6 (1%)	12	9
1	B	582/638 (91%)	547 (94%)	32 (6%)	3 (0%)	24	22
1	C	582/638 (91%)	557 (96%)	22 (4%)	3 (0%)	24	22
1	D	588/638 (92%)	557 (95%)	29 (5%)	2 (0%)	36	36
1	E	580/638 (91%)	555 (96%)	24 (4%)	1 (0%)	43	44
1	F	582/638 (91%)	556 (96%)	25 (4%)	1 (0%)	43	44
1	G	584/638 (92%)	551 (94%)	30 (5%)	3 (0%)	24	22
1	H	582/638 (91%)	554 (95%)	25 (4%)	3 (0%)	24	22
All	All	4660/5104 (91%)	4421 (95%)	217 (5%)	22 (0%)	24	22

All (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
1	A	342	LYS
1	B	342	LYS
1	C	342	LYS
1	E	342	LYS
1	F	342	LYS
1	G	342	LYS
1	A	59	LYS
1	D	59	LYS
1	D	342	LYS
1	H	342	LYS
1	H	623	HIS
1	A	353	ASP

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Mol	Chain	Res	Type
1	G	59	LYS
1	A	176	ALA
1	C	176	ALA
1	H	98	VAL
1	G	98	VAL

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%)	474 (95%)	23 (5%)	24	25
1	B	499/537 (93%)	475 (95%)	24 (5%)	23	23
1	C	499/537 (93%)	477 (96%)	22 (4%)	25	26
1	D	504/537 (94%)	479 (95%)	25 (5%)	22	22
1	E	497/537 (93%)	482 (97%)	15 (3%)	36	41
1	F	499/537 (93%)	481 (96%)	18 (4%)	31	34
1	G	501/537 (93%)	480 (96%)	21 (4%)	26	28
1	H	499/537 (93%)	477 (96%)	22 (4%)	25	26
All	All	3995/4296 (93%)	3825 (96%)	170 (4%)	26	27

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	78	HIS
1	A	85	LEU
1	A	125	ASN
1	A	269	ARG
1	A	270	ASN
1	A	275	VAL
1	A	276	VAL
1	A	314	LYS
1	A	353	ASP

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Mol	Chain	Res	Type
1	A	355	LEU
1	A	434	LEU
1	A	447	LYS
1	A	482	LYS
1	A	497	ILE
1	A	509	ILE
1	A	511	ASP
1	A	526	LYS
1	A	559	GLU
1	A	595	GLU
1	A	596	ILE
1	A	602	SER
1	A	632	ARG
1	B	78	HIS
1	B	85	LEU
1	B	125	ASN
1	B	128	CYS
1	B	148	ASN
1	B	158	ILE
1	B	275	VAL
1	B	276	VAL
1	B	297	ASP
1	B	311	LYS
1	B	313	SER
1	B	314	LYS
1	B	355	LEU
1	B	370	ILE
1	B	407	GLU
1	B	447	LYS
1	B	526	LYS
1	B	542	ASN
1	B	551	MET
1	B	559	GLU
1	B	575	ILE
1	B	576	ASP
1	B	595	GLU
1	B	596	ILE
1	C	59	LYS
1	C	60	ILE
1	C	78	HIS
1	C	85	LEU
1	C	125	ASN

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Mol	Chain	Res	Type
1	C	210	LEU
1	C	275	VAL
1	C	293	ILE
1	C	308	LYS
1	C	311	LYS
1	C	355	LEU
1	C	407	GLU
1	C	437	SER
1	C	447	LYS
1	C	458	ASP
1	C	482	LYS
1	C	497	ILE
1	C	505	LYS
1	C	526	LYS
1	C	558	GLN
1	C	596	ILE
1	C	620	TRP
1	D	60	ILE
1	D	78	HIS
1	D	85	LEU
1	D	125	ASN
1	D	148	ASN
1	D	207	VAL
1	D	210	LEU
1	D	225	GLU
1	D	255	CYS
1	D	275	VAL
1	D	293	ILE
1	D	311	LYS
1	D	314	LYS
1	D	355	LEU
1	D	397	ILE
1	D	407	GLU
1	D	417	LYS
1	D	447	LYS
1	D	497	ILE
1	D	511	ASP
1	D	526	LYS
1	D	542	ASN
1	D	558	GLN
1	D	596	ILE
1	D	620	TRP

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Mol	Chain	Res	Type
1	E	60	ILE
1	E	78	HIS
1	E	85	LEU
1	E	125	ASN
1	E	213	GLU
1	E	275	VAL
1	E	308	LYS
1	E	311	LYS
1	E	355	LEU
1	E	407	GLU
1	E	480	GLU
1	E	497	ILE
1	E	542	ASN
1	E	596	ILE
1	E	620	TRP
1	F	60	ILE
1	F	78	HIS
1	F	85	LEU
1	F	125	ASN
1	F	158	ILE
1	F	210	LEU
1	F	213[A]	GLU
1	F	213[B]	GLU
1	F	228	GLU
1	F	275	VAL
1	F	297	ASP
1	F	355	LEU
1	F	508	LYS
1	F	526	LYS
1	F	538	ILE
1	F	542	ASN
1	F	596	ILE
1	F	620	TRP
1	G	57	LYS
1	G	60	ILE
1	G	78	HIS
1	G	85	LEU
1	G	125	ASN
1	G	189	LYS
1	G	210	LEU
1	G	255	CYS
1	G	275	VAL

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Mol	Chain	Res	Type
1	G	313	SER
1	G	314	LYS
1	G	355	LEU
1	G	407	GLU
1	G	438	LEU
1	G	447	LYS
1	G	497	ILE
1	G	511	ASP
1	G	526	LYS
1	G	542	ASN
1	G	595	GLU
1	G	620	TRP
1	H	60	ILE
1	H	78	HIS
1	H	85	LEU
1	H	125	ASN
1	H	164	LYS
1	H	210	LEU
1	H	228	GLU
1	H	275	VAL
1	H	288	LYS
1	H	293	ILE
1	H	311	LYS
1	H	314	LYS
1	H	355	LEU
1	H	407	GLU
1	H	417	LYS
1	H	497	ILE
1	H	509	ILE
1	H	522	GLU
1	H	523	MET
1	H	526	LYS
1	H	596	ILE
1	H	620	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	79	GLN
1	A	111	ASN
1	A	125	ASN

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Mol	Chain	Res	Type
1	A	129	HIS
1	A	148	ASN
1	A	175	GLN
1	A	187	HIS
1	A	232	GLN
1	A	241	ASN
1	A	281	HIS
1	A	390	ASN
1	A	423	GLN
1	A	467	HIS
1	A	472	GLN
1	A	558	GLN
1	A	564	GLN
1	A	577	GLN
1	A	599	GLN
1	B	58	GLN
1	B	79	GLN
1	B	111	ASN
1	B	125	ASN
1	B	148	ASN
1	B	175	GLN
1	B	201	HIS
1	B	270	ASN
1	B	423	GLN
1	B	472	GLN
1	B	494	HIS
1	B	542	ASN
1	B	577	GLN
1	C	58	GLN
1	C	78	HIS
1	C	79	GLN
1	C	111	ASN
1	C	125	ASN
1	C	129	HIS
1	C	148	ASN
1	C	175	GLN
1	C	201	HIS
1	C	241	ASN
1	C	423	GLN
1	C	467	HIS
1	C	470	ASN
1	C	472	GLN

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Mol	Chain	Res	Type
1	C	494	HIS
1	C	558	GLN
1	C	577	GLN
1	D	58	GLN
1	D	79	GLN
1	D	111	ASN
1	D	115	HIS
1	D	125	ASN
1	D	129	HIS
1	D	148	ASN
1	D	175	GLN
1	D	201	HIS
1	D	214	ASN
1	D	232	GLN
1	D	423	GLN
1	D	472	GLN
1	D	542	ASN
1	D	558	GLN
1	D	577	GLN
1	E	58	GLN
1	E	79	GLN
1	E	111	ASN
1	E	125	ASN
1	E	129	HIS
1	E	148	ASN
1	E	175	GLN
1	E	201	HIS
1	E	241	ASN
1	E	423	GLN
1	E	472	GLN
1	E	542	ASN
1	E	558	GLN
1	E	577	GLN
1	F	58	GLN
1	F	79	GLN
1	F	111	ASN
1	F	125	ASN
1	F	129	HIS
1	F	148	ASN
1	F	175	GLN
1	F	201	HIS
1	F	241	ASN

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Mol	Chain	Res	Type
1	F	419	ASN
1	F	423	GLN
1	F	470	ASN
1	F	472	GLN
1	F	542	ASN
1	G	79	GLN
1	G	111	ASN
1	G	125	ASN
1	G	129	HIS
1	G	148	ASN
1	G	175	GLN
1	G	232	GLN
1	G	423	GLN
1	G	472	GLN
1	G	542	ASN
1	G	564	GLN
1	G	599	GLN
1	H	58	GLN
1	H	79	GLN
1	H	111	ASN
1	H	125	ASN
1	H	129	HIS
1	H	148	ASN
1	H	175	GLN
1	H	201	HIS
1	H	214	ASN
1	H	382	HIS
1	H	390	ASN
1	H	423	GLN
1	H	430	GLN
1	H	467	HIS
1	H	470	ASN
1	H	472	GLN
1	H	494	HIS
1	H	577	GLN
1	H	599	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	F	701	1	0,1,1	-	-	-		
2	CUA	B	701	1	0,1,1	-	-	-		
2	CUA	A	701	1	0,1,1	-	-	-		
3	CUK	G	702	1	0,6,6	-	-	-		
2	CUA	C	701	1	0,1,1	-	-	-		
3	CUK	C	702	1	0,6,6	-	-	-		
7	IMD	E	640	-	5,5,5	0.70	0	5,5,5	0.38	0
3	CUK	D	702	1	0,6,6	-	-	-		
3	CUK	E	702	1	0,6,6	-	-	-		
7	IMD	H	639	-	5,5,5	0.60	0	5,5,5	0.28	0
2	CUA	D	701	1	0,1,1	-	-	-		
2	CUA	H	701	1	0,1,1	-	-	-		
3	CUK	B	702	1	0,6,6	-	-	-		
7	IMD	G	639	-	5,5,5	0.74	0	5,5,5	0.51	0
7	IMD	E	639	-	5,5,5	0.67	0	5,5,5	0.35	0
3	CUK	F	702	1	0,6,6	-	-	-		
3	CUK	H	702	1	0,6,6	-	-	-		
7	IMD	F	639	-	5,5,5	0.60	0	5,5,5	0.57	0
3	CUK	A	702	1	0,6,6	-	-	-		
2	CUA	E	701	1	0,1,1	-	-	-		
7	IMD	D	639	-	5,5,5	0.65	0	5,5,5	0.35	0
2	CUA	G	701	1	0,1,1	-	-	-		

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	CUK	F	702	1	-	-	0/1/1/1
3	CUK	H	702	1	-	-	0/1/1/1
3	CUK	G	702	1	-	-	0/1/1/1
7	IMD	F	639	-	-	-	0/1/1/1
3	CUK	C	702	1	-	-	0/1/1/1
3	CUK	B	702	1	-	-	0/1/1/1
7	IMD	E	640	-	-	-	0/1/1/1
7	IMD	H	639	-	-	-	0/1/1/1
3	CUK	A	702	1	-	-	0/1/1/1
3	CUK	D	702	1	-	-	0/1/1/1
7	IMD	G	639	-	-	-	0/1/1/1
7	IMD	E	639	-	-	-	0/1/1/1
7	IMD	D	639	-	-	-	0/1/1/1
3	CUK	E	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.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	640	IMD	2	0
7	H	639	IMD	4	0
7	E	639	IMD	2	0
7	F	639	IMD	3	0
7	D	639	IMD	2	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	581/638 (91%)	0.08	3 (0%) 87 88	15, 33, 56, 70	1 (0%)
1	B	581/638 (91%)	0.05	2 (0%) 90 91	12, 33, 51, 62	3 (0%)
1	C	581/638 (91%)	-0.59	1 (0%) 91 92	8, 18, 31, 40	3 (0%)
1	D	588/638 (92%)	-0.48	0 100 100	9, 22, 36, 44	2 (0%)
1	E	581/638 (91%)	-0.69	0 100 100	8, 17, 29, 37	1 (0%)
1	F	581/638 (91%)	-0.63	0 100 100	9, 17, 31, 40	3 (0%)
1	G	585/638 (91%)	-0.43	1 (0%) 91 92	10, 22, 39, 50	1 (0%)
1	H	581/638 (91%)	-0.51	0 100 100	8, 20, 35, 45	3 (0%)
All	All	4659/5104 (91%)	-0.40	7 (0%) 91 92	8, 22, 43, 70	17 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	293	ILE	2.6
1	A	274	TRP	2.5
1	A	638	ALA	2.3
1	B	638	ALA	2.3
1	C	458	ASP	2.2
1	G	310	GLY	2.1
1	B	297	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	IMD	G	639	5/5	0.84	0.19	45,45,45,46	0
6	K	A	705	1/1	0.87	0.10	54,54,54,54	0
3	CUK	B	702	6/6	0.89	0.11	57,61,62,62	6
6	K	H	705	1/1	0.90	0.09	37,37,37,37	0
7	IMD	F	639	5/5	0.90	0.16	47,47,48,48	0
6	K	E	705	1/1	0.90	0.08	46,46,46,46	0
7	IMD	D	639	5/5	0.92	0.17	46,46,47,47	0
7	IMD	E	640	5/5	0.93	0.12	24,24,25,25	0
6	K	C	705	1/1	0.93	0.10	41,41,41,41	0
6	K	G	705	1/1	0.93	0.10	44,44,44,44	0
3	CUK	H	702	6/6	0.94	0.11	34,37,39,40	6
6	K	B	705	1/1	0.94	0.07	48,48,48,48	0
3	CUK	A	702	6/6	0.95	0.09	49,53,53,54	6
7	IMD	H	639	5/5	0.95	0.10	22,22,23,24	0
3	CUK	G	702	6/6	0.96	0.07	34,41,44,45	6
2	CUA	F	701	2/2	0.96	0.05	22,22,22,33	0
3	CUK	F	702	6/6	0.96	0.08	26,32,34,36	6
7	IMD	E	639	5/5	0.96	0.07	37,37,38,38	0
6	K	D	705	1/1	0.97	0.07	31,31,31,31	0
2	CUA	A	701	2/2	0.97	0.04	31,31,31,34	0
6	K	F	705	1/1	0.97	0.10	26,26,26,26	0
2	CUA	G	701	2/2	0.97	0.04	19,19,19,27	0
2	CUA	B	701	2/2	0.97	0.04	52,52,52,54	0
4	CA	A	703	1/1	0.97	0.04	47,47,47,47	0
5	CL	A	704	1/1	0.97	0.11	46,46,46,46	0
5	CL	B	704	1/1	0.97	0.10	50,50,50,50	0
2	CUA	C	701	2/2	0.97	0.04	27,27,27,33	0
3	CUK	C	702	6/6	0.97	0.08	29,36,38,39	6
3	CUK	E	702	6/6	0.97	0.08	31,37,40,41	6
2	CUA	E	701	2/2	0.98	0.03	18,18,18,24	0
2	CUA	H	701	2/2	0.98	0.03	33,33,33,35	0
3	CUK	D	702	6/6	0.98	0.07	27,34,36,38	6
2	CUA	D	701	2/2	0.98	0.03	21,21,21,23	0
4	CA	D	703	1/1	0.99	0.02	25,25,25,25	0
5	CL	C	704	1/1	0.99	0.07	26,26,26,26	0
5	CL	D	704	1/1	0.99	0.10	25,25,25,25	0
5	CL	E	704	1/1	0.99	0.05	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	G	704	1/1	0.99	0.06	29,29,29,29	0
5	CL	H	704	1/1	0.99	0.10	29,29,29,29	0
4	CA	E	703	1/1	0.99	0.02	18,18,18,18	0
4	CA	G	703	1/1	0.99	0.04	26,26,26,26	0
4	CA	H	703	1/1	0.99	0.02	15,15,15,15	0
4	CA	B	703	1/1	0.99	0.02	27,27,27,27	0
4	CA	C	703	1/1	1.00	0.01	15,15,15,15	0
5	CL	F	704	1/1	1.00	0.08	24,24,24,24	0
4	CA	F	703	1/1	1.00	0.02	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.