



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:00 AM UTC

PDB ID : 3SBR / pdb_00003sbr
Title : Pseudomonas stutzeri nitrous oxide reductase, P1 crystal form with substrate
Authors : Pomowski, A.; Zumft, W.G.; Kroneck, P.M.H.; Einsle, O.
Deposited on : 2011-06-06
Resolution : 2.24 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

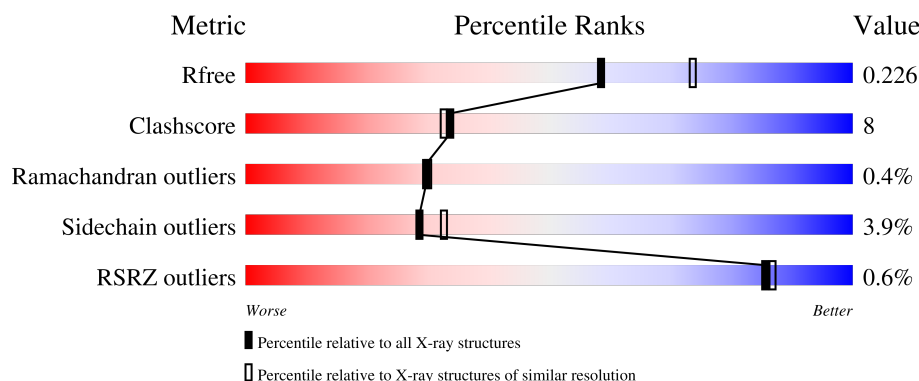
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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% 76% 13% 9%
1	B	638	1% 74% 15% 9%
1	C	638	12% 78% 9%
1	D	638	13% 78% 8%
1	E	638	13% 76% 9%

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Mol	Chain	Length	Quality of chain
1	F	638	
1	G	638	
1	H	638	

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
5	CL	A	704	-	-	X	-
7	IMD	H	639	-	-	X	-

2 Entry composition

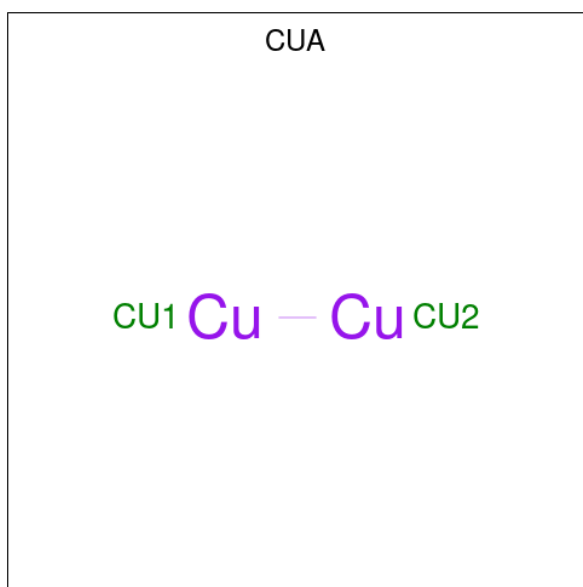
There are 9 unique types of molecules in this entry. The entry contains 39507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

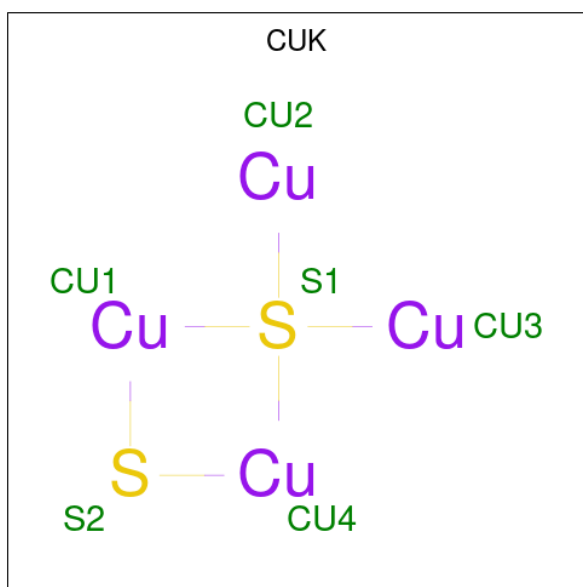
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	1	0
			4573	2891	788	862	32			
1	B	581	Total	C	N	O	S	0	3	0
			4592	2902	792	866	32			
1	C	581	Total	C	N	O	S	0	3	0
			4590	2900	790	868	32			
1	D	588	Total	C	N	O	S	0	2	0
			4636	2929	799	876	32			
1	E	581	Total	C	N	O	S	0	1	0
	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

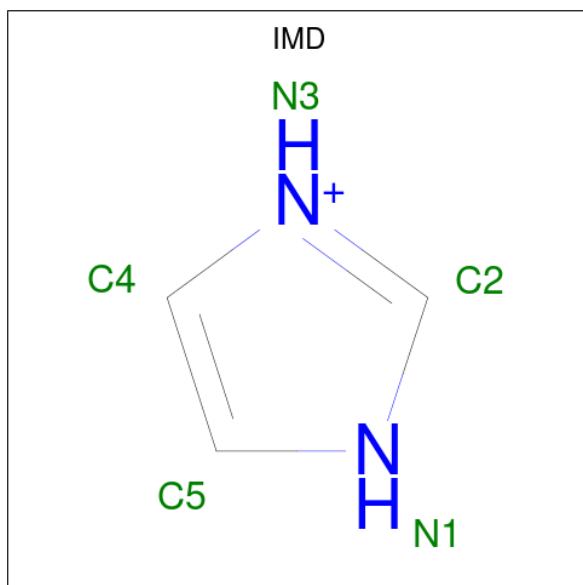
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	K 1	0	0
6	B	1	Total 1	K 1	0	0
6	C	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	E	1	Total 1	K 1	0	0

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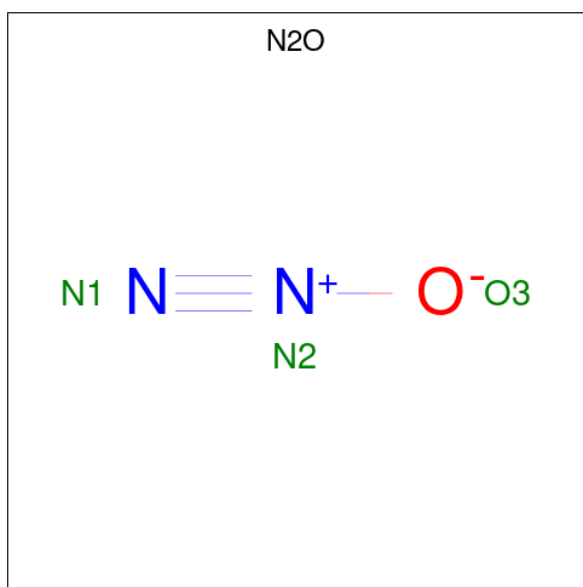
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total K 1 1	0	0
6	G	1	Total K 1 1	0	0
6	H	1	Total K 1 1	0	0

- 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 NITROUS OXIDE (CCD ID: N2O) (formula: N_2O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	N	O	0	0
			3	2	1		
8	H	1	Total	N	O	0	0
			3	2	1		

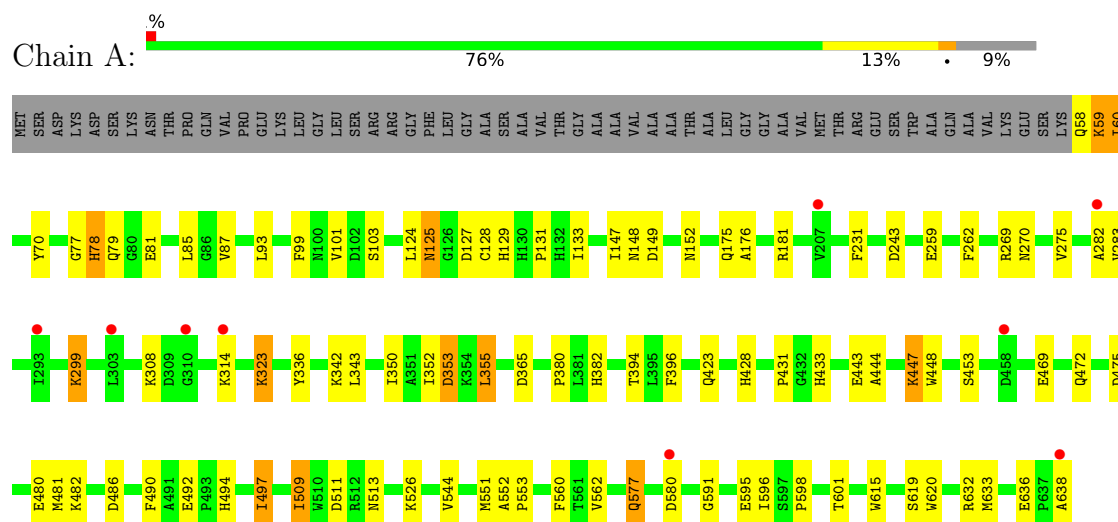
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	207	Total	O	0	0
			207	207		
9	B	183	Total	O	0	0
			183	183		
9	C	367	Total	O	0	0
			367	367		
9	D	365	Total	O	0	0
			365	365		
9	E	393	Total	O	0	0
			393	393		
9	F	411	Total	O	0	0
			411	411		
9	G	349	Total	O	0	0
			349	349		
9	H	353	Total	O	0	0
			353	353		

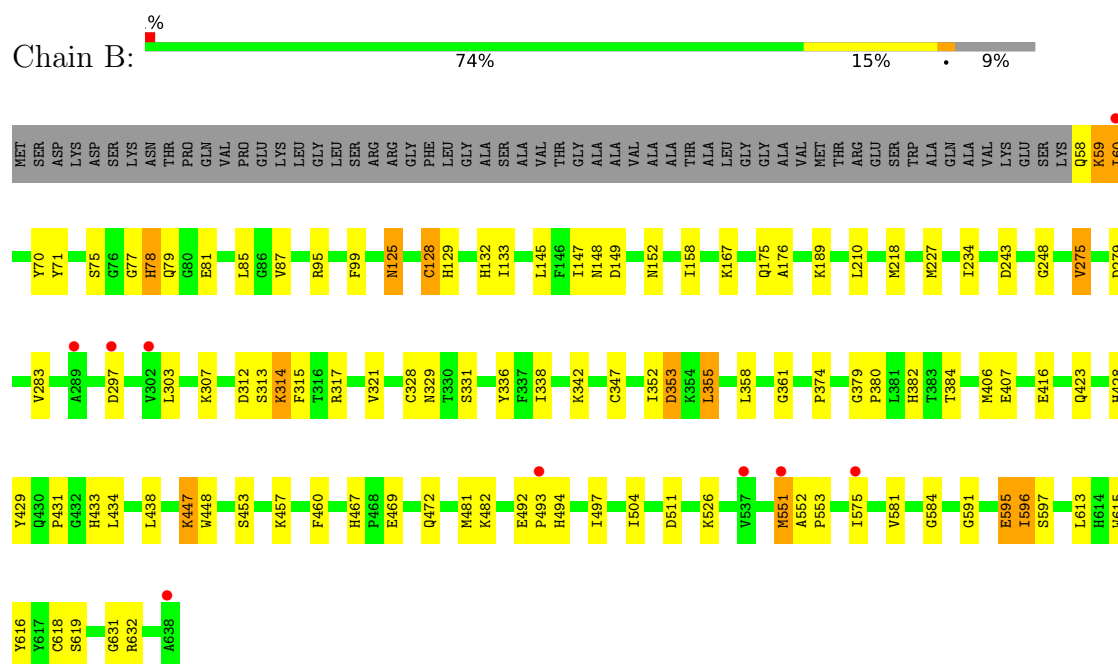
3 Residue-property plots [i](#)

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

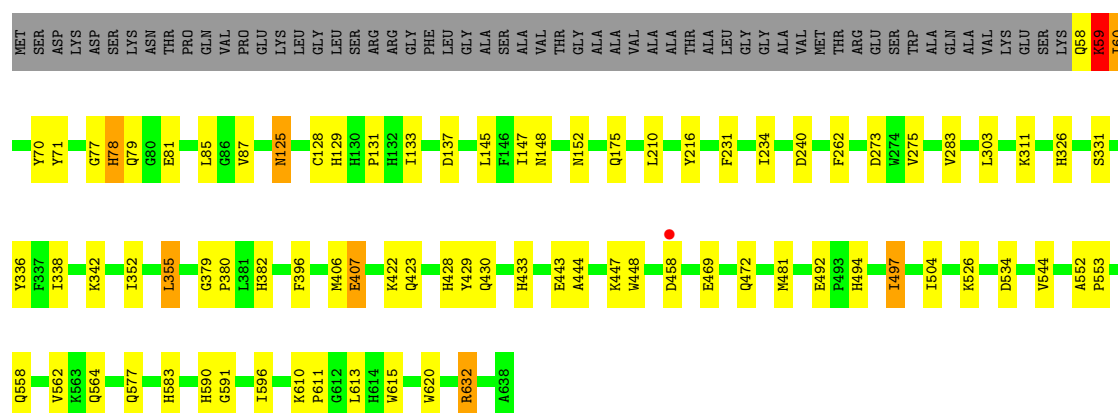


• Molecule 1: Nitrous-oxide reductase



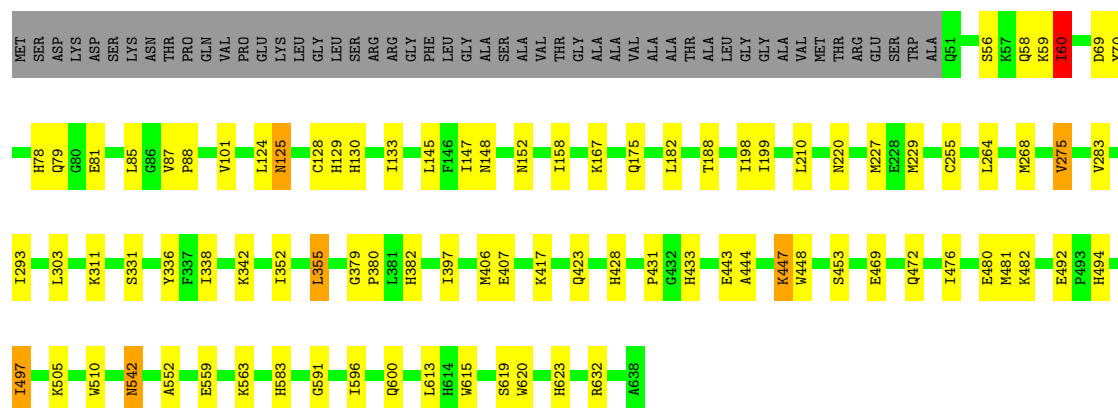
• Molecule 1: Nitrous-oxide reductase

Chain C:  78% 12% 9%



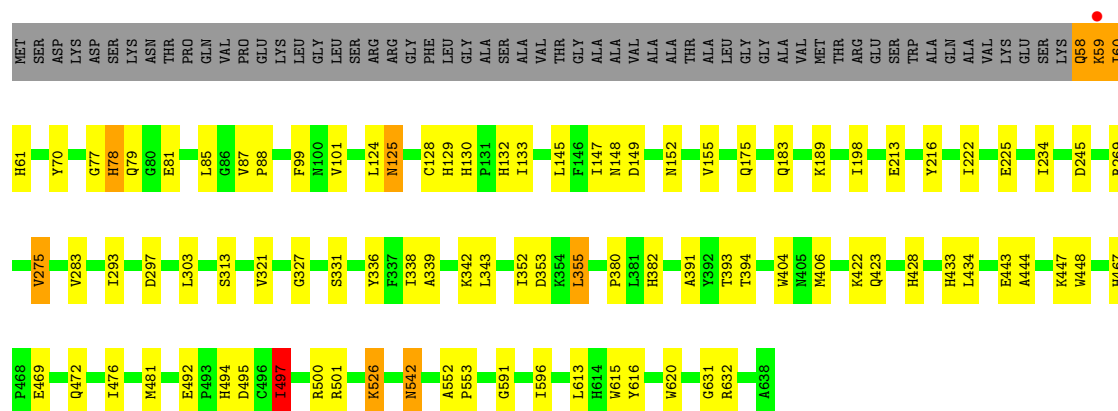
• Molecule 1: Nitrous-oxide reductase

Chain D:  78% 13% 8%



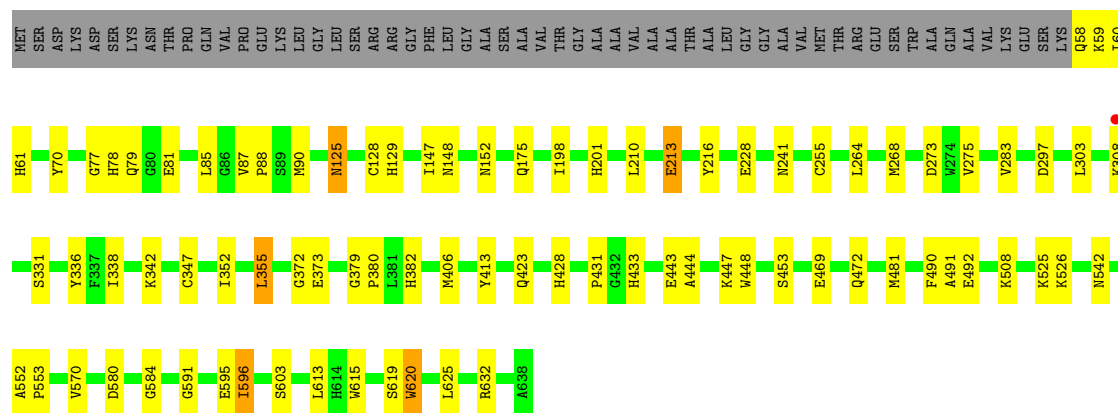
• Molecule 1: Nitrous-oxide reductase

Chain E:  76% 13% 9%

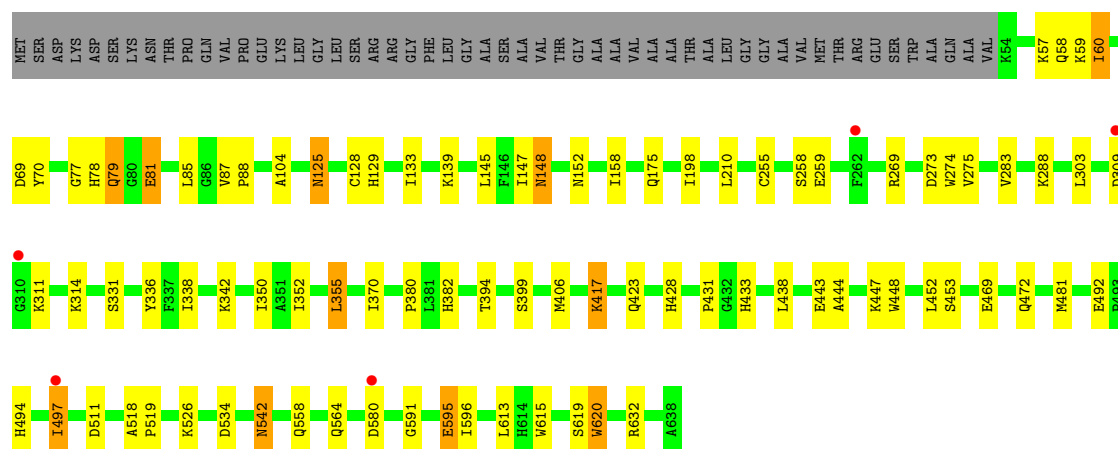
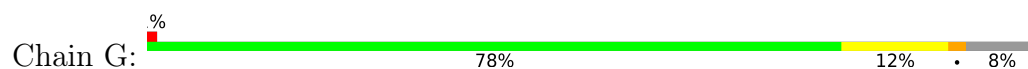


• Molecule 1: Nitrous-oxide reductase

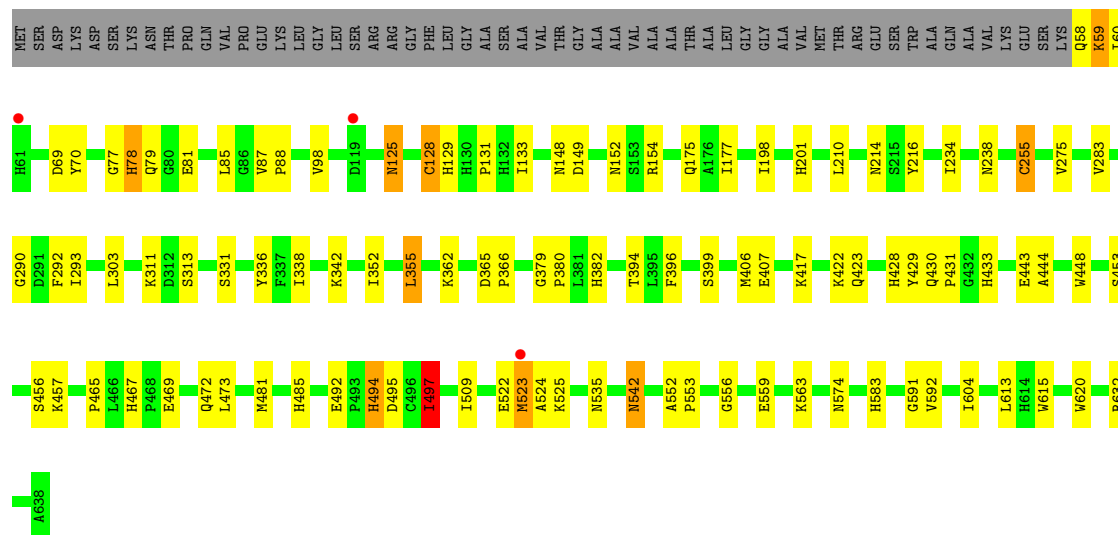
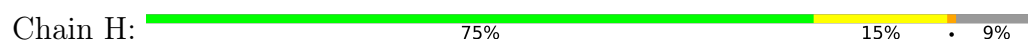
Chain F:  78% 12% 9%



• 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, α , β , γ	96.58Å 106.45Å 130.88Å 111.45° 107.22° 90.72°	Depositor
Resolution (Å)	95.00 – 2.24 95.00 – 2.24	Depositor EDS
% Data completeness (in resolution range)	93.3 (95.00-2.24) 93.3 (95.00-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.89 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.173 , 0.227 0.174 , 0.226	Depositor DCC
R_{free} test set	10299 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	39507	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.37% 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: CA, CL, CUK, IMD, CUA, N2O, K

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	0.58	1/4685 (0.0%)	0.84	5/6345 (0.1%)
1	B	0.60	0/4705	0.82	1/6372 (0.0%)
1	C	0.69	0/4702	0.86	2/6368 (0.0%)
1	D	0.64	0/4748	0.83	2/6428 (0.0%)
1	E	0.72	0/4687	0.89	4/6348 (0.1%)
1	F	0.68	0/4705	0.85	1/6372 (0.0%)
1	G	0.67	1/4718 (0.0%)	0.85	2/6387 (0.0%)
1	H	0.69	0/4702	0.86	4/6368 (0.1%)
All	All	0.66	2/37652 (0.0%)	0.85	21/50988 (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	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	273	ASP	CA-C	-5.76	1.50	1.53
1	A	60	ILE	CA-CB	5.17	1.61	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	ASP	N-CA-C	-6.54	103.42	108.78
1	E	497	ILE	CB-CA-C	-5.94	100.44	110.71
1	C	534	ASP	N-CA-C	5.69	119.19	110.20
1	A	336	TYR	N-CA-C	5.61	118.24	108.76
1	A	60	ILE	N-CA-C	5.58	120.95	109.34
1	E	59	LYS	N-CA-C	5.53	122.58	110.80
1	G	273	ASP	N-CA-C	-5.50	104.27	108.78
1	H	494	HIS	N-CA-C	-5.50	104.20	111.96
1	A	59	LYS	N-CA-C	5.47	122.46	110.80
1	H	336	TYR	N-CA-C	5.46	118.36	109.24
1	H	59	LYS	N-CA-C	5.38	122.26	110.80
1	D	275	VAL	N-CA-CB	5.36	117.42	110.99
1	D	199	ILE	N-CA-C	5.33	115.03	109.01
1	H	497	ILE	CB-CA-C	-5.20	102.50	110.50
1	A	636	GLU	CA-C-N	5.19	126.32	119.84
1	A	636	GLU	C-N-CA	5.19	126.32	119.84
1	B	581	VAL	N-CA-C	5.17	111.74	106.21
1	G	534	ASP	N-CA-C	5.13	118.31	110.20
1	E	225	GLU	N-CA-C	5.05	116.60	111.14
1	E	353	ASP	N-CA-C	5.05	118.21	111.75
1	F	273	ASP	N-CA-C	-5.03	104.66	108.78

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	58	GLN	Peptide
1	E	58	GLN	Peptide
1	F	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	62	0
1	B	4592	0	4452	85	0
1	C	4590	0	4449	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4636	0	4505	69	0
1	E	4575	0	4440	85	0
1	F	4593	0	4450	70	0
1	G	4606	0	4478	76	0
1	H	4590	0	4449	80	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	1	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	1	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	2	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
5	D	1	0	0	0	0
5	E	1	0	0	1	0
5	F	1	0	0	1	0
5	G	1	0	0	0	0
5	H	1	0	0	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
7	G	5	0	5	2	0
7	H	5	0	5	4	0
8	D	3	0	0	1	0
8	H	3	0	0	0	0
9	A	207	0	0	3	0
9	B	183	0	0	5	0
9	C	367	0	0	4	0
9	D	365	0	0	7	0
9	E	393	0	0	9	0
9	F	411	0	0	7	0
9	G	349	0	0	9	0
9	H	353	0	0	5	0
All	All	39507	0	35694	557	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 (557) 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:E:338:ILE:HD11	1:E:406:MET:HE3	1.22	1.17
1:F:338:ILE:HD11	1:F:406:MET:HE3	1.20	1.12
1:B:338:ILE:HD11	1:B:406:MET:HE3	1.31	1.10
1:H:338:ILE:HD11	1:H:406:MET:CE	1.80	1.10
1:C:338:ILE:HD11	1:C:406:MET:HE3	1.31	1.06
9:D:2328:HOH:O	1:E:542:ASN:HB3	1.58	1.03
1:H:338:ILE:HD11	1:H:406:MET:HE3	1.40	1.02
1:H:338:ILE:CD1	1:H:406:MET:HE3	1.94	0.97
1:E:336:TYR:CD2	1:E:406:MET:HE2	1.99	0.97
1:H:469:GLU:HG3	1:H:492:GLU:HA	1.48	0.95
1:C:469:GLU:HG3	1:C:492:GLU:HA	1.48	0.95
1:G:423:GLN:HE22	1:G:481:MET:H	1.10	0.93
1:C:423:GLN:HE22	1:C:481:MET:H	1.13	0.93
1:B:423:GLN:HE22	1:B:481:MET:H	1.15	0.93
1:G:331:SER:HB3	1:G:406:MET:HE1	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:GLN:HE22	1:A:481:MET:H	1.18	0.92
1:A:259:GLU:HG2	1:A:269:ARG:HB3	1.53	0.91
1:G:125:ASN:HD21	1:H:591:GLY:HA2	1.36	0.90
1:E:423:GLN:HE22	1:E:481:MET:H	1.13	0.90
1:C:564:GLN:OE1	1:C:611:PRO:HG3	1.72	0.90
1:B:469:GLU:HG3	1:B:492:GLU:HA	1.51	0.90
1:D:423:GLN:HE22	1:D:481:MET:H	1.16	0.89
1:D:338:ILE:HD11	1:D:406:MET:HE3	1.55	0.88
1:G:283:VAL:HG13	1:G:303:LEU:HD13	1.56	0.88
1:G:288:LYS:HG2	9:G:1278:HOH:O	1.73	0.87
1:G:417:LYS:HG3	9:G:2993:HOH:O	1.75	0.86
1:H:283:VAL:HG13	1:H:303:LEU:HD13	1.56	0.86
1:A:125:ASN:HD21	1:B:591:GLY:HA2	1.41	0.85
1:D:283:VAL:HG13	1:D:303:LEU:HD13	1.58	0.85
1:G:469:GLU:HG3	1:G:492:GLU:HA	1.58	0.84
1:E:336:TYR:HD2	1:E:406:MET:HE2	1.39	0.84
1:G:331:SER:CB	1:G:406:MET:HE1	2.08	0.84
1:E:269:ARG:HD2	9:E:820:HOH:O	1.75	0.84
1:E:469:GLU:HG3	1:E:492:GLU:HA	1.58	0.84
1:C:129:HIS:H	1:C:148:ASN:HD21	1.24	0.84
1:B:283:VAL:HG13	1:B:303:LEU:HD13	1.59	0.83
1:F:423:GLN:HE22	1:F:481:MET:H	1.21	0.83
1:F:469:GLU:HG3	1:F:492:GLU:HA	1.61	0.82
1:D:336:TYR:HD2	1:D:406:MET:HE2	1.43	0.82
1:H:525:LYS:HD3	9:H:2817:HOH:O	1.77	0.82
1:F:338:ILE:HD11	1:F:406:MET:CE	2.08	0.82
1:B:352:ILE:HA	1:B:355:LEU:HD22	1.62	0.81
1:F:382:HIS:CE1	1:F:433:HIS:CE1	2.67	0.81
1:D:336:TYR:CD2	1:D:406:MET:HE2	2.15	0.81
1:H:423:GLN:HE22	1:H:481:MET:H	1.29	0.81
1:G:129:HIS:H	1:G:148:ASN:HD21	1.29	0.80
1:E:428:HIS:H	1:E:472:GLN:HE22	1.27	0.80
1:B:133:ILE:HG13	1:B:497:ILE:HD12	1.63	0.79
3:C:702:CUK:S1	8:D:640:N2O:N1	2.56	0.79
1:E:331:SER:HB3	1:E:406:MET:HE1	1.64	0.79
1:E:283:VAL:HG13	1:E:303:LEU:HD13	1.65	0.79
1:E:336:TYR:HD2	1:E:406:MET:CE	1.94	0.79
1:D:331:SER:HB3	1:D:406:MET:HE1	1.65	0.78
1:E:125:ASN:HD21	1:F:591:GLY:HA2	1.46	0.78
1:E:338:ILE:CD1	1:E:406:MET:HE3	2.09	0.78
1:A:352:ILE:HA	1:A:355:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:LYS:HE2	1:E:88:PRO:HG3	1.63	0.78
1:D:129:HIS:H	1:D:148:ASN:HD21	1.29	0.78
1:F:336:TYR:CD2	1:F:406:MET:HE2	2.19	0.77
1:C:382:HIS:CE1	1:C:433:HIS:CE1	2.72	0.77
1:F:428:HIS:H	1:F:472:GLN:HE22	1.33	0.76
1:E:382:HIS:HB3	9:E:1097:HOH:O	1.86	0.76
1:B:407:GLU:HG3	9:B:2163:HOH:O	1.86	0.76
1:F:283:VAL:HG13	1:F:303:LEU:HD13	1.68	0.76
1:G:428:HIS:H	1:G:472:GLN:HE22	1.34	0.75
1:B:551:MET:HB2	1:B:575:ILE:HD11	1.69	0.75
1:C:352:ILE:HA	1:C:355:LEU:HD22	1.68	0.75
1:C:458:ASP:HB3	9:C:737:HOH:O	1.87	0.74
1:F:129:HIS:H	1:F:148:ASN:HD21	1.34	0.74
1:C:407:GLU:HG2	1:H:563:LYS:HD3	1.70	0.74
1:E:591:GLY:HA2	1:F:125:ASN:HD21	1.52	0.73
1:C:137:ASP:HB3	9:C:1790:HOH:O	1.89	0.73
1:E:59:LYS:NZ	1:E:448:TRP:HE1	1.86	0.73
1:H:59:LYS:HE2	1:H:88:PRO:HG3	1.70	0.73
1:H:382:HIS:NE2	1:H:433:HIS:CD2	2.57	0.72
1:C:336:TYR:CD2	1:C:406:MET:HE2	2.24	0.72
1:E:133:ILE:HG13	1:E:497:ILE:HD13	1.72	0.72
1:E:336:TYR:CD2	1:E:406:MET:CE	2.72	0.72
1:D:352:ILE:HA	1:D:355:LEU:HD22	1.70	0.71
1:D:336:TYR:HD2	1:D:406:MET:CE	2.03	0.71
1:G:336:TYR:HD2	1:G:406:MET:CE	2.03	0.71
1:G:591:GLY:HA2	1:H:125:ASN:HD21	1.54	0.71
1:H:428:HIS:H	1:H:472:GLN:HE22	1.38	0.71
1:D:469:GLU:HG3	1:D:492:GLU:HA	1.71	0.71
1:F:352:ILE:HA	1:F:355:LEU:HD22	1.72	0.71
1:G:338:ILE:HD11	1:G:406:MET:HE3	1.72	0.71
1:E:428:HIS:H	1:E:472:GLN:NE2	1.89	0.71
1:G:198:ILE:H	7:G:639:IMD:H4	1.55	0.71
1:C:283:VAL:HG13	1:C:303:LEU:CD1	2.21	0.71
1:C:613:LEU:HD11	1:C:632:ARG:HB3	1.72	0.71
1:D:428:HIS:H	1:D:472:GLN:HE22	1.36	0.70
1:F:198:ILE:H	7:F:639:IMD:H2	1.57	0.70
1:E:70:TYR:HB2	1:E:87:VAL:HB	1.75	0.69
1:H:59:LYS:HZ1	1:H:448:TRP:HE1	1.40	0.68
1:E:129:HIS:H	1:E:148:ASN:HD21	1.40	0.68
1:H:129:HIS:H	1:H:148:ASN:HD21	1.41	0.68
1:C:591:GLY:HA2	1:D:125:ASN:HD21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:338:ILE:CD1	1:H:406:MET:CE	2.60	0.68
1:C:331:SER:HB3	1:C:406:MET:HE1	1.76	0.67
1:C:125:ASN:HD21	1:D:591:GLY:HA2	1.60	0.67
1:H:331:SER:HB3	1:H:406:MET:HE1	1.76	0.67
1:B:331:SER:HB3	1:B:406:MET:HE1	1.76	0.67
1:B:382[A]:HIS:CE1	1:B:433:HIS:NE2	2.62	0.67
1:C:338:ILE:CD1	1:C:406:MET:HE3	2.17	0.67
1:C:552:ALA:HB2	1:C:583:HIS:HE1	1.60	0.67
1:D:542:ASN:HB3	9:D:654:HOH:O	1.94	0.66
1:H:382:HIS:CE1	1:H:433:HIS:NE2	2.63	0.66
1:D:59:LYS:HE3	1:D:69:ASP:OD2	1.96	0.66
1:A:129:HIS:H	1:A:148:ASN:HD21	1.42	0.66
1:H:59:LYS:NZ	1:H:448:TRP:HE1	1.92	0.66
1:B:382[A]:HIS:NE2	1:B:433:HIS:CD2	2.63	0.66
1:A:175:GLN:HE22	1:B:615:TRP:H	1.44	0.65
1:A:70:TYR:HB2	1:A:87:VAL:HB	1.79	0.65
1:G:336:TYR:CD2	1:G:406:MET:HE2	2.32	0.65
1:G:615:TRP:CZ2	7:H:639:IMD:H4	2.33	0.64
1:B:314:LYS:HD2	9:B:2644:HOH:O	1.97	0.64
1:G:336:TYR:HD2	1:G:406:MET:HE2	1.63	0.64
1:E:59:LYS:CE	1:E:88:PRO:HG3	2.28	0.64
1:H:59:LYS:HE3	1:H:69:ASP:OD2	1.98	0.64
1:B:317:ARG:HG3	1:B:358:LEU:HG	1.79	0.64
1:H:431:PRO:HA	1:H:453:SER:HA	1.79	0.63
1:B:133:ILE:HG13	1:B:497:ILE:CD1	2.29	0.63
1:G:615:TRP:CH2	7:H:639:IMD:H4	2.33	0.63
1:B:129:HIS:H	1:B:148:ASN:HD21	1.45	0.63
1:E:125:ASN:ND2	1:F:591:GLY:HA2	2.13	0.63
1:A:125:ASN:ND2	1:B:591:GLY:HA2	2.11	0.63
1:B:59:LYS:O	1:B:60:ILE:HG22	1.99	0.62
1:A:299:LYS:HD3	9:A:2452:HOH:O	2.00	0.62
1:D:632:ARG:HD3	9:D:2130:HOH:O	1.98	0.62
1:H:283:VAL:HG13	1:H:303:LEU:CD1	2.29	0.62
1:A:580:ASP:OD1	1:B:467:HIS:HB2	2.00	0.62
1:E:331:SER:CB	1:E:406:MET:HE1	2.29	0.62
1:E:382:HIS:NE2	1:E:433:HIS:CD2	2.68	0.62
1:H:382:HIS:NE2	1:H:433:HIS:NE2	2.48	0.62
1:C:336:TYR:HD2	1:C:406:MET:HE2	1.65	0.62
1:E:591:GLY:HA2	1:F:125:ASN:ND2	2.15	0.62
1:E:382:HIS:CE1	1:E:433:HIS:NE2	2.67	0.62
1:H:128:CYS:HB3	1:H:148:ASN:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:SER:CB	1:D:406:MET:HE1	2.28	0.61
1:D:423:GLN:HE22	1:D:481:MET:N	1.95	0.61
1:H:382:HIS:CE1	1:H:433:HIS:CE1	2.89	0.61
1:D:129:HIS:H	1:D:148:ASN:ND2	1.97	0.61
1:D:613:LEU:HD11	1:D:632:ARG:HG2	1.81	0.61
1:A:591:GLY:HA2	1:B:125:ASN:HD21	1.66	0.61
1:G:423:GLN:HE22	1:G:481:MET:N	1.91	0.60
1:A:469:GLU:HG3	1:A:492:GLU:HA	1.82	0.60
1:E:59:LYS:O	1:E:60:ILE:HG23	2.01	0.60
1:B:382[B]:HIS:HD2	1:B:434:LEU:HD23	1.67	0.60
1:C:129:HIS:H	1:C:148:ASN:ND2	1.98	0.60
1:D:70:TYR:HB2	1:D:87:VAL:HB	1.84	0.60
1:C:59:LYS:HZ1	1:C:448:TRP:HE1	1.50	0.60
1:B:428:HIS:H	1:B:472:GLN:HE22	1.49	0.59
1:G:632:ARG:HD3	9:G:2045:HOH:O	2.02	0.59
1:B:70:TYR:HB2	1:B:87:VAL:HB	1.83	0.59
1:A:382:HIS:CE1	1:A:433:HIS:CE1	2.91	0.59
1:D:79:GLN:HE22	1:D:81:GLU:CG	2.16	0.59
1:F:59:LYS:NZ	1:F:448:TRP:HE1	2.01	0.59
1:G:125:ASN:ND2	1:H:591:GLY:HA2	2.12	0.59
1:G:382:HIS:CE1	1:G:433:HIS:CE1	2.90	0.59
1:H:592:VAL:HG13	1:H:604:ILE:HD13	1.83	0.58
1:A:423:GLN:HE22	1:A:481:MET:N	1.97	0.58
1:A:262:PHE:HB2	1:B:632:ARG:HD2	1.84	0.58
1:E:428:HIS:N	1:E:472:GLN:HE22	2.00	0.58
1:B:429:TYR:CD1	1:B:457:LYS:HD2	2.38	0.58
1:C:407:GLU:HG2	1:H:563:LYS:CD	2.31	0.58
1:G:595:GLU:HG2	1:G:596:ILE:N	2.19	0.58
1:F:336:TYR:CD2	1:F:406:MET:CE	2.87	0.58
1:G:615:TRP:H	1:H:175:GLN:HE22	1.52	0.58
1:H:352:ILE:HA	1:H:355:LEU:HD22	1.84	0.58
1:E:447:LYS:HD3	9:E:2352:HOH:O	2.03	0.57
1:A:382:HIS:CE1	5:A:704:CL:CL	2.94	0.57
1:E:615:TRP:H	1:F:175:GLN:HE22	1.51	0.57
1:E:61:HIS:HB3	9:F:1215:HOH:O	2.05	0.57
1:F:148:ASN:H	1:F:148:ASN:HD22	1.51	0.57
1:B:133:ILE:CG1	1:B:497:ILE:HD12	2.34	0.57
1:C:137:ASP:CB	9:C:1790:HOH:O	2.49	0.57
1:F:59:LYS:HZ1	1:F:448:TRP:HE1	1.52	0.57
1:A:99:PHE:CE2	1:A:149:ASP:HB2	2.39	0.56
1:C:59:LYS:NZ	1:C:448:TRP:HE1	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ILE:HD11	1:C:406:MET:CE	2.22	0.56
1:F:336:TYR:HD2	1:F:406:MET:CE	2.17	0.56
1:G:591:GLY:HA2	1:H:125:ASN:ND2	2.20	0.56
1:F:70:TYR:HB2	1:F:87:VAL:HB	1.87	0.56
1:E:382:HIS:NE2	1:E:433:HIS:NE2	2.53	0.56
1:F:331:SER:HB3	1:F:406:MET:HE1	1.87	0.56
1:F:336:TYR:HD2	1:F:406:MET:HE2	1.68	0.56
1:D:382:HIS:CE1	1:D:433:HIS:CE1	2.94	0.56
1:C:128:CYS:HB3	1:C:148:ASN:O	2.05	0.56
1:E:59:LYS:HZ1	1:E:448:TRP:HE1	1.52	0.56
1:G:129:HIS:H	1:G:148:ASN:ND2	2.01	0.56
1:H:133:ILE:HG13	1:H:497:ILE:HD13	1.86	0.56
1:B:79:GLN:HE22	1:B:81:GLU:CG	2.19	0.55
1:F:428:HIS:H	1:F:472:GLN:NE2	2.03	0.55
1:B:469:GLU:CG	1:B:492:GLU:HA	2.31	0.55
1:D:59:LYS:O	1:D:60:ILE:HG23	2.07	0.55
1:B:379:GLY:N	1:B:380:PRO:HD3	2.22	0.55
1:C:423:GLN:HE22	1:C:481:MET:N	1.95	0.55
1:A:544:VAL:HG21	1:A:562:VAL:HG12	1.88	0.55
1:G:619:SER:O	1:H:78:HIS:CE1	2.60	0.55
1:H:423:GLN:HE22	1:H:481:MET:N	2.03	0.55
1:H:428:HIS:H	1:H:472:GLN:NE2	2.03	0.54
1:D:542:ASN:HD22	1:D:542:ASN:C	2.14	0.54
1:D:128:CYS:HB2	1:D:147:ILE:HG12	1.90	0.54
1:H:201:HIS:HE1	1:H:216:TYR:O	1.90	0.54
1:A:78:HIS:CE1	1:B:619:SER:O	2.61	0.54
1:E:494:HIS:HE1	9:F:1431:HOH:O	1.89	0.54
1:H:399[B]:SER:HB2	1:H:430:GLN:H	1.73	0.54
1:A:131:PRO:O	1:A:497:ILE:HG12	2.08	0.54
1:E:175:GLN:HE22	1:F:615:TRP:H	1.56	0.54
1:E:338:ILE:HD11	1:E:406:MET:CE	2.15	0.54
1:C:591:GLY:HA2	1:D:125:ASN:ND2	2.23	0.54
1:F:90:MET:HG3	9:F:2183:HOH:O	2.07	0.54
1:H:198:ILE:H	7:H:639:IMD:HN3	1.56	0.54
1:F:632:ARG:HD3	9:F:1451:HOH:O	2.07	0.54
1:H:542:ASN:HB3	9:H:1267:HOH:O	2.07	0.54
1:A:125:ASN:ND2	1:A:152:ASN:HD21	2.05	0.54
1:C:175:GLN:HE22	1:D:615:TRP:H	1.55	0.54
1:F:77:GLY:HA2	1:F:128:CYS:O	2.08	0.54
1:G:70:TYR:HB2	1:G:87:VAL:HB	1.89	0.54
1:G:469:GLU:CG	1:G:492:GLU:HA	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:447:LYS:HE2	9:F:2850:HOH:O	2.08	0.53
1:G:564:GLN:HG2	9:G:2944:HOH:O	2.07	0.53
1:E:613:LEU:HD11	1:E:632:ARG:HG2	1.89	0.53
1:B:338:ILE:HD11	1:B:406:MET:CE	2.21	0.53
1:G:129:HIS:N	1:G:148:ASN:HD21	2.04	0.53
1:C:231:PHE:CE1	1:C:283:VAL:HG11	2.43	0.53
1:C:336:TYR:HD2	1:C:406:MET:CE	2.22	0.53
1:D:79:GLN:HE22	1:D:81:GLU:HG2	1.74	0.52
1:B:382[B]:HIS:CD2	1:B:434:LEU:H	2.27	0.52
1:C:145:LEU:HD11	1:C:497:ILE:HD11	1.91	0.52
1:G:352:ILE:HA	1:G:355:LEU:HD22	1.91	0.52
1:E:352:ILE:HA	1:E:355:LEU:HD22	1.91	0.52
1:G:428:HIS:H	1:G:472:GLN:NE2	2.06	0.52
1:C:125:ASN:ND2	1:C:152:ASN:HD21	2.07	0.52
1:E:632:ARG:HD3	9:E:2177:HOH:O	2.09	0.52
1:G:497:ILE:HB	9:G:675:HOH:O	2.10	0.52
1:A:511:ASP:HB3	1:A:513:ASN:OD1	2.10	0.52
1:B:77:GLY:HA2	1:B:128:CYS:O	2.10	0.52
1:B:382[A]:HIS:CD2	1:B:433:HIS:CD2	2.98	0.52
1:G:497:ILE:CG2	9:G:675:HOH:O	2.58	0.52
1:A:428:HIS:H	1:A:472:GLN:HE22	1.58	0.51
1:G:59:LYS:HE3	1:G:88:PRO:HG3	1.91	0.51
1:H:365:ASP:OD1	1:H:366:PRO:HD2	2.11	0.51
1:G:175:GLN:HE22	1:H:615:TRP:H	1.57	0.51
1:C:125:ASN:ND2	1:D:591:GLY:HA2	2.24	0.51
1:D:59:LYS:HE2	1:D:88:PRO:HG3	1.92	0.51
1:D:264:LEU:HG	1:D:268:MET:HE2	1.93	0.51
1:H:523:MET:HG3	1:H:524:ALA:N	2.24	0.51
1:A:431:PRO:HA	1:A:453:SER:HA	1.93	0.51
1:E:99:PHE:CE2	1:E:149:ASP:HB2	2.45	0.51
1:G:258:SER:HB2	1:G:274:TRP:CZ3	2.45	0.51
1:D:428:HIS:H	1:D:472:GLN:NE2	2.07	0.51
1:C:331:SER:CB	1:C:406:MET:HE1	2.41	0.51
1:E:382:HIS:CD2	1:E:433:HIS:CD2	2.99	0.51
1:F:443:GLU:O	1:F:444:ALA:C	2.54	0.51
1:C:428:HIS:H	1:C:472:GLN:HE22	1.58	0.50
1:G:198:ILE:H	7:G:639:IMD:C4	2.22	0.50
1:A:282:ALA:HB1	1:A:314:LYS:HD2	1.93	0.50
1:C:615:TRP:H	1:D:175:GLN:HE22	1.57	0.50
1:B:382[A]:HIS:NE2	1:B:433:HIS:NE2	2.58	0.50
1:D:129:HIS:CE1	1:D:494:HIS:CE1	2.98	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:HIS:CE1	1:A:494:HIS:CE1	2.99	0.50
1:D:129:HIS:N	1:D:148:ASN:HD21	2.04	0.50
1:E:129:HIS:H	1:E:148:ASN:ND2	2.07	0.50
1:C:443:GLU:O	1:C:444:ALA:C	2.55	0.50
1:D:382:HIS:CE1	1:D:433:HIS:NE2	2.79	0.50
1:H:79:GLN:HE22	1:H:81:GLU:CG	2.25	0.50
1:F:79:GLN:HE22	1:F:81:GLU:CG	2.25	0.50
1:F:198:ILE:H	7:F:639:IMD:C2	2.23	0.50
1:F:613:LEU:HD11	1:F:632:ARG:HG2	1.92	0.50
1:G:59:LYS:NZ	1:G:448:TRP:HE1	2.09	0.50
1:B:336:TYR:CD2	1:B:406:MET:HE2	2.47	0.49
1:C:615:TRP:HD1	1:D:175:GLN:NE2	2.10	0.49
1:E:382:HIS:CE1	5:E:704:CL:CL	3.03	0.49
1:E:467:HIS:HB2	1:F:580:ASP:OD1	2.12	0.49
1:E:433:HIS:ND1	1:E:495:ASP:CG	2.70	0.49
1:F:338:ILE:CD1	1:F:406:MET:HE3	2.15	0.49
1:G:283:VAL:CG1	1:G:303:LEU:HD13	2.35	0.49
1:C:615:TRP:CH2	7:D:639:IMD:H2	2.47	0.49
1:E:101:VAL:HG21	1:E:124:LEU:HD22	1.93	0.49
1:A:129:HIS:N	1:A:148:ASN:HD21	2.10	0.49
1:C:133:ILE:HG13	1:C:497:ILE:HD13	1.95	0.49
1:C:79:GLN:HE22	1:C:81:GLU:CG	2.24	0.49
1:A:128:CYS:HB2	1:A:147:ILE:HG12	1.95	0.49
1:H:429:TYR:CD2	1:H:457:LYS:HD2	2.48	0.49
1:A:509:ILE:HG22	1:A:598:PRO:HB2	1.94	0.48
1:E:125:ASN:ND2	1:E:152:ASN:HD21	2.11	0.48
1:F:423:GLN:NE2	1:F:481:MET:H	2.01	0.48
1:H:58:GLN:HG2	1:H:59:LYS:HD3	1.94	0.48
1:E:79:GLN:HE22	1:E:81:GLU:CG	2.26	0.48
9:G:1326:HOH:O	1:H:465:PRO:HD2	2.12	0.48
1:A:125:ASN:HD21	1:A:152:ASN:HD21	1.62	0.48
1:F:128:CYS:HB2	1:F:147:ILE:CD1	2.43	0.48
1:F:382:HIS:HB3	9:F:2403:HOH:O	2.12	0.48
1:C:433:HIS:HB2	1:C:494:HIS:O	2.14	0.48
1:E:155:VAL:HG21	1:E:222:ILE:CD1	2.44	0.48
1:F:129:HIS:H	1:F:148:ASN:ND2	2.06	0.48
1:B:125:ASN:HD21	1:B:152:ASN:HD21	1.61	0.48
1:B:307:LYS:HG2	1:B:312:ASP:HA	1.95	0.48
1:F:431:PRO:HA	1:F:453:SER:HA	1.95	0.48
1:H:382:HIS:CD2	1:H:433:HIS:CD2	3.01	0.48
1:B:613:LEU:HD11	1:B:632:ARG:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:131:PRO:O	1:H:497:ILE:HG12	2.13	0.48
1:F:428:HIS:N	1:F:472:GLN:HE22	2.08	0.48
1:F:125:ASN:ND2	1:F:152:ASN:HD21	2.12	0.48
1:F:128:CYS:HB3	1:F:148:ASN:O	2.13	0.48
1:F:490:PHE:CD2	1:F:491:ALA:HB2	2.49	0.48
1:A:619:SER:O	1:B:78:HIS:CE1	2.67	0.48
1:E:433:HIS:HB2	1:E:494:HIS:O	2.14	0.48
1:F:213[A]:GLU:O	1:F:213[A]:GLU:HG3	2.13	0.48
1:G:133:ILE:HG13	1:G:497:ILE:CD1	2.44	0.48
1:C:262:PHE:HB2	1:D:632:ARG:HD2	1.96	0.47
1:G:336:TYR:CD2	1:G:406:MET:CE	2.88	0.47
1:F:264:LEU:HG	1:F:268:MET:HE2	1.96	0.47
1:D:431:PRO:HA	1:D:453:SER:HA	1.97	0.47
1:D:510:TRP:CD1	1:D:600:GLN:HB2	2.50	0.47
1:A:79:GLN:HE22	1:A:81:GLU:CG	2.27	0.47
1:C:396:PHE:CE1	1:C:430:GLN:HB3	2.50	0.47
9:D:2328:HOH:O	7:E:639:IMD:H4	2.14	0.47
1:G:613:LEU:HD11	1:G:632:ARG:HG2	1.96	0.47
1:D:552:ALA:HB2	1:D:583:HIS:HE1	1.80	0.47
1:G:148:ASN:HD22	1:G:148:ASN:H	1.61	0.47
1:H:428:HIS:N	1:H:472:GLN:HE22	2.09	0.47
7:H:639:IMD:H5	9:H:686:HOH:O	2.15	0.47
1:A:78:HIS:HA	1:A:127:ASP:HA	1.97	0.47
1:B:595:GLU:OE2	1:B:597:SER:OG	2.23	0.47
1:D:559:GLU:HA	1:D:632:ARG:O	2.15	0.47
1:E:443:GLU:O	1:E:444:ALA:C	2.57	0.47
1:F:128:CYS:HB2	1:F:147:ILE:HD11	1.97	0.47
1:H:469:GLU:CG	1:H:492:GLU:HA	2.33	0.47
1:A:58:GLN:HE22	1:A:447:LYS:HG2	1.79	0.47
1:A:323:LYS:HG2	1:A:343:LEU:HB2	1.96	0.47
1:B:59:LYS:NZ	1:B:448:TRP:HE1	2.11	0.47
1:B:243:ASP:HB2	1:B:328:CYS:O	2.15	0.47
1:C:77:GLY:HA2	1:C:128:CYS:O	2.15	0.47
1:E:382:HIS:CE1	1:E:433:HIS:CE1	3.03	0.47
1:F:347:CYS:O	1:F:373:GLU:HA	2.15	0.47
1:F:379:GLY:N	1:F:380:PRO:HD3	2.30	0.47
1:F:595:GLU:HB2	1:F:620:TRP:CZ3	2.50	0.47
1:G:431:PRO:HA	1:G:453:SER:HA	1.97	0.47
1:A:59:LYS:NZ	1:A:448:TRP:HE1	2.13	0.47
1:A:314:LYS:HB2	9:A:1084:HOH:O	2.15	0.47
1:B:353:ASP:HB2	9:B:2008:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:GLY:HA2	9:B:1868:HOH:O	2.14	0.47
1:C:78:HIS:CE1	1:D:619:SER:O	2.68	0.47
1:D:59:LYS:NZ	1:D:448:TRP:HE1	2.13	0.47
1:D:198:ILE:H	7:D:639:IMD:HN1	1.62	0.47
1:E:394:THR:HG23	1:E:434:LEU:HD22	1.97	0.47
1:H:396:PHE:CE1	1:H:430:GLN:HB3	2.49	0.47
1:B:75:SER:O	1:B:493:PRO:HB3	2.16	0.46
1:C:590:HIS:CE1	1:C:610:LYS:HE2	2.50	0.46
1:F:595:GLU:HG2	1:F:596:ILE:N	2.29	0.46
1:H:380:PRO:HA	1:H:394:THR:O	2.15	0.46
1:H:433:HIS:HB2	1:H:494:HIS:O	2.15	0.46
1:H:149:ASP:HB3	1:H:154:ARG:HB2	1.97	0.46
1:H:214:ASN:ND2	9:H:742:HOH:O	2.48	0.46
1:B:128:CYS:HB2	1:B:147:ILE:HD11	1.97	0.46
1:C:148:ASN:HD22	1:C:148:ASN:H	1.64	0.46
1:F:372:GLY:HA2	1:F:413:TYR:HB2	1.98	0.46
1:B:347:CYS:O	1:B:374:PRO:HD2	2.15	0.46
1:B:429:TYR:CE1	1:B:457:LYS:HD2	2.50	0.46
1:D:148:ASN:H	1:D:148:ASN:HD22	1.63	0.46
1:E:469:GLU:CG	1:E:492:GLU:HA	2.38	0.46
1:C:125:ASN:HD21	1:C:152:ASN:HD21	1.64	0.46
1:G:350:ILE:HG12	1:G:370:ILE:HD13	1.97	0.46
1:G:399[B]:SER:O	1:G:399[B]:SER:OG	2.31	0.46
1:G:452:LEU:HD22	1:G:494:HIS:O	2.16	0.46
1:A:129:HIS:H	1:A:148:ASN:ND2	2.10	0.46
1:A:560:PHE:CE2	1:A:633:MET:HG3	2.51	0.46
1:E:129:HIS:N	1:E:148:ASN:HD21	2.11	0.46
1:F:59:LYS:HE2	1:F:88:PRO:HG3	1.98	0.46
1:A:577:GLN:HE21	1:A:577:GLN:HB3	1.56	0.46
1:C:336:TYR:CD2	1:C:406:MET:CE	2.97	0.46
1:E:130:HIS:H	1:E:148:ASN:ND2	2.14	0.46
1:B:148:ASN:H	1:B:148:ASN:HD22	1.64	0.46
1:G:59:LYS:HZ1	1:G:448:TRP:HE1	1.64	0.46
1:H:433:HIS:HD2	3:H:702:CUK:S2	2.39	0.46
1:D:125:ASN:H	1:D:125:ASN:HD22	1.64	0.45
1:G:309:ASP:C	1:G:311:LYS:H	2.25	0.45
1:C:145:LEU:CD1	1:C:497:ILE:HD11	2.45	0.45
1:D:443:GLU:O	1:D:444:ALA:C	2.59	0.45
1:H:238:ASN:O	1:H:255:CYS:HB2	2.16	0.45
1:H:613:LEU:HD11	1:H:632:ARG:HB3	1.99	0.45
1:D:128:CYS:HB3	1:D:148:ASN:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:433:HIS:ND1	1:H:495:ASP:CG	2.74	0.45
1:A:396:PHE:HA	1:A:431:PRO:HD2	1.97	0.45
1:G:125:ASN:ND2	1:G:152:ASN:HD21	2.14	0.45
1:H:443:GLU:O	1:H:444:ALA:C	2.58	0.45
1:D:447:LYS:HE3	9:D:2098:HOH:O	2.16	0.45
1:E:58:GLN:N	9:E:1461:HOH:O	2.48	0.45
1:G:125:ASN:HD22	1:G:125:ASN:H	1.63	0.45
1:H:473:LEU:HB3	1:H:485:HIS:HB3	1.99	0.45
1:D:101:VAL:HG21	1:D:124:LEU:HD22	1.98	0.45
1:B:428:HIS:H	1:B:472:GLN:NE2	2.14	0.45
1:B:433:HIS:HB2	1:B:494:HIS:O	2.16	0.45
1:E:500:ARG:O	1:E:501:ARG:C	2.59	0.45
1:F:148:ASN:H	1:F:148:ASN:ND2	2.15	0.45
1:H:125:ASN:ND2	1:H:152:ASN:HD21	2.14	0.45
1:C:422:LYS:HA	1:C:422:LYS:HD3	1.83	0.45
1:A:615:TRP:H	1:B:175:GLN:HE22	1.66	0.44
1:A:638:ALA:HA	9:A:1042:HOH:O	2.17	0.44
1:C:70:TYR:HB2	1:C:87:VAL:HB	1.97	0.44
1:D:336:TYR:CD2	1:D:406:MET:CE	2.89	0.44
1:E:58:GLN:CG	1:E:59:LYS:HD3	2.48	0.44
1:D:379:GLY:N	1:D:380:PRO:HD3	2.32	0.44
1:A:93:LEU:HD22	1:B:460:PHE:HB3	1.99	0.44
1:A:101:VAL:HG21	1:A:124:LEU:HD22	1.98	0.44
1:B:275:VAL:HG13	1:B:321:VAL:HG21	1.99	0.44
1:C:216:TYR:CD1	1:C:234:ILE:HG23	2.52	0.44
1:D:59:LYS:NZ	9:D:708:HOH:O	2.46	0.44
1:E:77:GLY:HA2	1:E:128:CYS:O	2.18	0.44
1:E:128:CYS:HB3	1:E:148:ASN:O	2.18	0.44
1:E:198:ILE:H	7:E:640:IMD:HN1	1.64	0.44
1:E:327:GLY:O	1:E:339:ALA:HA	2.18	0.44
1:B:125:ASN:ND2	1:B:152:ASN:HD21	2.14	0.44
1:G:59:LYS:O	1:G:60:ILE:HG23	2.18	0.44
1:G:139:LYS:HG2	1:G:443:GLU:HG3	1.98	0.44
1:G:145:LEU:HD12	1:G:497:ILE:HD11	2.00	0.44
1:G:615:TRP:H	1:H:175:GLN:NE2	2.15	0.44
1:H:148:ASN:HD22	1:H:148:ASN:H	1.65	0.44
1:A:133:ILE:HG13	1:A:497:ILE:HD13	2.00	0.44
1:A:480:GLU:OE1	1:F:526:LYS:HE3	2.17	0.44
1:H:552:ALA:HA	1:H:553:PRO:HA	1.81	0.44
1:A:472:GLN:HG2	1:A:486:ASP:OD1	2.18	0.44
1:B:279:ASP:O	1:B:283:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:VAL:HG13	1:C:303:LEU:HD13	1.98	0.44
1:G:438:LEU:HB2	1:G:444:ALA:HA	2.00	0.44
1:B:99:PHE:CE2	1:B:149:ASP:HB2	2.53	0.44
1:B:431:PRO:HA	1:B:453:SER:HA	1.99	0.44
1:G:558:GLN:NE2	9:G:695:HOH:O	2.49	0.44
1:B:59:LYS:HB3	1:B:60:ILE:H	1.46	0.43
1:C:544:VAL:HG21	1:C:562:VAL:HG12	1.99	0.43
1:F:490:PHE:CE2	1:F:491:ALA:HB2	2.53	0.43
1:G:59:LYS:CE	1:G:88:PRO:HG3	2.48	0.43
1:A:380:PRO:HA	1:A:394:THR:O	2.17	0.43
1:F:213[A]:GLU:O	1:F:213[A]:GLU:CG	2.65	0.43
1:G:380:PRO:HA	1:G:394:THR:O	2.18	0.43
1:A:103:SER:HB2	1:B:125:ASN:HA	2.00	0.43
1:A:181:ARG:HD2	1:A:243:ASP:CG	2.43	0.43
1:B:595:GLU:HG2	1:B:596:ILE:N	2.34	0.43
1:C:428:HIS:H	1:C:472:GLN:NE2	2.16	0.43
1:E:216:TYR:CD1	1:E:234:ILE:HG23	2.54	0.43
1:E:245:ASP:OD1	1:E:245:ASP:C	2.59	0.43
1:F:128:CYS:HB2	1:F:147:ILE:HG12	2.00	0.43
1:A:128:CYS:HB3	1:A:148:ASN:O	2.18	0.43
1:C:613:LEU:CD1	1:C:632:ARG:HB3	2.45	0.43
1:D:125:ASN:ND2	1:D:152:ASN:HD21	2.16	0.43
1:H:379:GLY:N	1:H:380:PRO:HD3	2.34	0.43
1:H:535:ASN:OD1	1:H:556:GLY:HA3	2.17	0.43
1:H:574:ASN:ND2	1:H:583:HIS:CD2	2.86	0.43
1:C:71:TYR:CE1	1:C:504:ILE:HB	2.54	0.43
1:G:497:ILE:HG21	9:G:675:HOH:O	2.17	0.43
1:E:78:HIS:ND1	9:E:1432:HOH:O	2.35	0.43
1:E:382:HIS:CG	9:E:1097:HOH:O	2.72	0.43
1:C:494:HIS:HE1	9:C:1439:HOH:O	2.02	0.43
1:D:145:LEU:CD1	1:D:497:ILE:HD11	2.49	0.43
1:E:616:TYR:CE1	1:E:631:GLY:HA3	2.54	0.43
1:H:362:LYS:NZ	9:H:715:HOH:O	2.52	0.43
1:D:552:ALA:HB1	1:D:623:HIS:HB2	2.00	0.43
1:H:216:TYR:CD1	1:H:234:ILE:HG23	2.54	0.42
1:A:382:HIS:HE1	5:A:704:CL:CL	2.39	0.42
1:B:71:TYR:CE2	1:B:504:ILE:HB	2.54	0.42
1:E:476:ILE:HG22	1:E:481:MET:HG2	2.01	0.42
1:B:303:LEU:HD22	1:B:315:PHE:CZ	2.53	0.42
1:E:59:LYS:HZ3	1:E:448:TRP:HE1	1.63	0.42
1:E:275:VAL:CG1	1:E:321:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:HIS:HD2	9:F:1448:HOH:O	2.01	0.42
1:F:201:HIS:HE1	1:F:216:TYR:O	2.03	0.42
1:B:58:GLN:HE22	1:B:447:LYS:HG2	1.84	0.42
1:B:329:ASN:HD21	1:B:382[B]:HIS:CE1	2.38	0.42
1:E:391:ALA:HB3	1:E:404:TRP:CE2	2.54	0.42
1:G:77:GLY:HA2	1:G:128:CYS:O	2.19	0.42
1:G:128:CYS:HB2	1:G:147:ILE:HG12	2.02	0.42
1:G:259:GLU:HG2	1:G:269:ARG:HB3	2.01	0.42
1:H:77:GLY:HA2	1:H:128:CYS:O	2.19	0.42
1:H:422:LYS:HA	1:H:422:LYS:HD3	1.82	0.42
1:B:552:ALA:HA	1:B:553:PRO:HA	1.73	0.42
1:D:133:ILE:HG13	1:D:497:ILE:CD1	2.49	0.42
1:B:382[B]:HIS:HD2	1:B:434:LEU:H	1.68	0.42
1:B:613:LEU:CD1	1:B:632:ARG:HB3	2.50	0.42
1:C:552:ALA:HA	1:C:553:PRO:HA	1.82	0.42
1:E:128:CYS:HB2	1:E:147:ILE:HG12	2.02	0.42
1:C:58:GLN:HG2	1:C:59:LYS:HD3	2.02	0.42
1:C:469:GLU:CG	1:C:492:GLU:HA	2.34	0.42
1:D:480:GLU:OE1	1:E:526:LYS:HE2	2.19	0.42
1:E:183:GLN:OE1	1:E:189:LYS:HB3	2.20	0.42
1:F:125:ASN:HD21	1:F:152:ASN:HD21	1.68	0.42
1:H:338:ILE:HD11	1:H:406:MET:HE1	1.90	0.42
1:C:428:HIS:HA	1:C:429:TYR:CG	2.55	0.42
1:D:59:LYS:C	1:D:60:ILE:HG23	2.45	0.42
1:D:130:HIS:H	1:D:148:ASN:ND2	2.17	0.42
1:D:167:LYS:CB	1:D:227:MET:HG3	2.50	0.42
7:E:640:IMD:H2	1:F:615:TRP:CZ2	2.54	0.42
1:C:175:GLN:NE2	1:D:615:TRP:H	2.17	0.42
1:C:240:ASP:OD2	1:C:326:HIS:ND1	2.51	0.42
1:B:616:TYR:CE1	1:B:631:GLY:HA3	2.55	0.41
1:F:570:VAL:O	1:F:603:SER:HA	2.21	0.41
1:F:584:GLY:HA3	1:F:619:SER:OG	2.19	0.41
1:G:542:ASN:C	1:G:542:ASN:HD22	2.28	0.41
1:B:79:GLN:HE21	1:B:79:GLN:HB3	1.61	0.41
1:C:379:GLY:N	1:C:380:PRO:HD3	2.35	0.41
1:G:104:ALA:O	1:G:620:TRP:HZ3	2.04	0.41
1:G:175:GLN:NE2	1:H:615:TRP:HD1	2.18	0.41
1:H:382:HIS:CE1	5:H:704:CL:CL	3.10	0.41
1:A:58:GLN:HB3	1:A:475:ASP:OD2	2.19	0.41
1:E:552:ALA:HA	1:E:553:PRO:HA	1.84	0.41
1:H:290:GLY:HA2	1:H:292:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:HIS:O	1:E:145:LEU:HA	2.20	0.41
1:A:591:GLY:HA2	1:B:125:ASN:ND2	2.33	0.41
1:B:283:VAL:CG1	1:B:303:LEU:HD13	2.40	0.41
1:D:505:LYS:HD2	9:D:744:HOH:O	2.20	0.41
1:G:59:LYS:CE	1:G:69:ASP:OD2	2.69	0.41
1:G:79:GLN:HE22	1:G:81:GLU:CG	2.33	0.41
1:A:490:PHE:CD2	1:B:95:ARG:HD2	2.55	0.41
1:B:167:LYS:CB	1:B:227:MET:HG3	2.50	0.41
1:E:382:HIS:CB	9:E:1097:HOH:O	2.56	0.41
1:A:551:MET:O	1:A:552:ALA:C	2.64	0.41
1:B:125:ASN:HD22	1:B:125:ASN:H	1.68	0.41
1:E:343:LEU:HD21	1:F:625:LEU:HD21	2.02	0.41
1:E:382:HIS:O	1:E:393:THR:HA	2.21	0.41
1:C:131:PRO:O	1:C:497:ILE:HG12	2.21	0.41
1:C:382:HIS:CE1	5:C:704:CL:CL	3.11	0.41
1:D:56:SER:H	1:D:482:LYS:NZ	2.19	0.41
1:E:422:LYS:HA	1:E:422:LYS:HD3	1.91	0.41
9:E:2589:HOH:O	1:F:61:HIS:HB3	2.21	0.41
1:F:241:ASN:ND2	5:F:704:CL:CL	2.91	0.41
1:F:552:ALA:HA	1:F:553:PRO:HA	1.86	0.41
1:G:331:SER:HB3	1:G:406:MET:CE	2.35	0.41
1:H:70:TYR:HB2	1:H:87:VAL:HB	2.03	0.41
1:H:148:ASN:HB2	1:H:177:ILE:HG22	2.03	0.41
1:A:443:GLU:O	1:A:444:ALA:C	2.64	0.41
1:C:128:CYS:HB2	1:C:147:ILE:CD1	2.51	0.41
1:D:182:LEU:HB3	1:D:188:THR:HG23	2.03	0.41
1:E:380:PRO:HA	1:E:394:THR:O	2.21	0.41
7:E:640:IMD:H2	1:F:615:TRP:CH2	2.56	0.41
1:B:338:ILE:CD1	1:B:406:MET:HE3	2.23	0.40
1:B:382[B]:HIS:CD2	1:B:434:LEU:HD23	2.52	0.40
1:B:384:THR:HG22	1:B:434:LEU:HG	2.02	0.40
1:B:584:GLY:O	1:B:618:CYS:HA	2.21	0.40
1:D:476:ILE:HG22	1:D:481:MET:HG2	2.01	0.40
1:G:518:ALA:N	1:G:519:PRO:CD	2.84	0.40
1:G:580:ASP:OD1	1:H:467:HIS:HB2	2.21	0.40
1:A:231:PHE:CE1	1:A:283:VAL:HG11	2.57	0.40
1:B:129:HIS:N	1:B:148:ASN:HD21	2.14	0.40
1:B:132:HIS:O	1:B:145:LEU:HA	2.21	0.40
1:B:248:GLY:HA2	9:B:2425:HOH:O	2.21	0.40
1:G:336:TYR:HA	1:G:350:ILE:O	2.22	0.40
1:G:433:HIS:HB2	1:G:494:HIS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:HG2	1:A:59:LYS:HB2	2.04	0.40
1:B:218:MET:HG2	1:B:234:ILE:HA	2.04	0.40
1:C:133:ILE:HG13	1:C:497:ILE:CD1	2.51	0.40
1:D:220:ASN:HB3	1:D:229:MET:HE1	2.03	0.40
1:E:542:ASN:HD22	1:E:542:ASN:H	1.70	0.40
1:G:129:HIS:CE1	1:G:494:HIS:CE1	3.09	0.40
1:H:456:SER:O	1:H:457:LYS:C	2.63	0.40
1:A:77:GLY:HA2	1:A:128:CYS:O	2.21	0.40
1:A:552:ALA:HA	1:A:553:PRO:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	32 (6%)	4 (1%)	18	16
1	B	582/638 (91%)	554 (95%)	24 (4%)	4 (1%)	18	16
1	C	582/638 (91%)	560 (96%)	19 (3%)	3 (0%)	24	23
1	D	588/638 (92%)	561 (95%)	25 (4%)	2 (0%)	36	38
1	E	580/638 (91%)	555 (96%)	24 (4%)	1 (0%)	43	48
1	F	582/638 (91%)	552 (95%)	27 (5%)	3 (0%)	24	23
1	G	584/638 (92%)	556 (95%)	27 (5%)	1 (0%)	43	48
1	H	582/638 (91%)	557 (96%)	23 (4%)	2 (0%)	36	38
All	All	4660/5104 (91%)	4439 (95%)	201 (4%)	20 (0%)	30	30

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	60	ILE

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Mol	Chain	Res	Type
1	B	342	LYS
1	C	59	LYS
1	A	342	LYS
1	E	342	LYS
1	F	342	LYS
1	H	342	LYS
1	A	353	ASP
1	B	59	LYS
1	C	342	LYS
1	D	342	LYS
1	G	342	LYS
1	A	308	LYS
1	B	176	ALA
1	F	213[A]	GLU
1	F	213[B]	GLU
1	A	176	ALA
1	D	60	ILE
1	H	98	VAL
1	C	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%)	474 (95%)	23 (5%)	24	25
1	B	499/537 (93%)	477 (96%)	22 (4%)	25	27
1	C	499/537 (93%)	481 (96%)	18 (4%)	31	36
1	D	504/537 (94%)	484 (96%)	20 (4%)	28	32
1	E	497/537 (93%)	482 (97%)	15 (3%)	36	43
1	F	499/537 (93%)	483 (97%)	16 (3%)	34	40
1	G	501/537 (93%)	479 (96%)	22 (4%)	25	27
1	H	499/537 (93%)	478 (96%)	21 (4%)	26	29
All	All	3995/4296 (93%)	3838 (96%)	157 (4%)	28	33

All (157) 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	270	ASN
1	A	275	VAL
1	A	299	LYS
1	A	323	LYS
1	A	350	ILE
1	A	353	ASP
1	A	355	LEU
1	A	365	ASP
1	A	447	LYS
1	A	482	LYS
1	A	497	ILE
1	A	509	ILE
1	A	526	LYS
1	A	577	GLN
1	A	595	GLU
1	A	596	ILE
1	A	601	THR
1	A	620	TRP
1	A	632	ARG
1	B	78	HIS
1	B	85	LEU
1	B	125	ASN
1	B	128	CYS
1	B	158	ILE
1	B	189	LYS
1	B	210	LEU
1	B	275	VAL
1	B	297	ASP
1	B	313	SER
1	B	314	LYS
1	B	353	ASP
1	B	355	LEU
1	B	416	GLU
1	B	438	LEU
1	B	447	LYS
1	B	482	LYS
1	B	511	ASP
1	B	526	LYS

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Mol	Chain	Res	Type
1	B	551	MET
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
1	C	210	LEU
1	C	275	VAL
1	C	311	LYS
1	C	355	LEU
1	C	407	GLU
1	C	447	LYS
1	C	497	ILE
1	C	526	LYS
1	C	558	GLN
1	C	577	GLN
1	C	596	ILE
1	C	620	TRP
1	C	632	ARG
1	D	60	ILE
1	D	78	HIS
1	D	85	LEU
1	D	125	ASN
1	D	158	ILE
1	D	210	LEU
1	D	255	CYS
1	D	275	VAL
1	D	293	ILE
1	D	311	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	542	ASN
1	D	563	LYS
1	D	596	ILE
1	D	620	TRP
1	E	60	ILE

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Mol	Chain	Res	Type
1	E	78	HIS
1	E	85	LEU
1	E	125	ASN
1	E	213	GLU
1	E	275	VAL
1	E	293	ILE
1	E	297	ASP
1	E	313	SER
1	E	355	LEU
1	E	497	ILE
1	E	526	LYS
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	210	LEU
1	F	228	GLU
1	F	255	CYS
1	F	275	VAL
1	F	297	ASP
1	F	308	LYS
1	F	355	LEU
1	F	508	LYS
1	F	525	LYS
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	79	GLN
1	G	81	GLU
1	G	85	LEU
1	G	125	ASN
1	G	148	ASN
1	G	158	ILE
1	G	210	LEU
1	G	255	CYS
1	G	275	VAL

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Mol	Chain	Res	Type
1	G	314	LYS
1	G	355	LEU
1	G	417	LYS
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	128	CYS
1	H	210	LEU
1	H	255	CYS
1	H	275	VAL
1	H	293	ILE
1	H	311	LYS
1	H	313	SER
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	542	ASN
1	H	559	GLU
1	H	620	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	78	HIS
1	A	79	GLN
1	A	111	ASN
1	A	125	ASN
1	A	129	HIS
1	A	148	ASN

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	201	HIS
1	A	232	GLN
1	A	281	HIS
1	A	382	HIS
1	A	423	GLN
1	A	430	GLN
1	A	472	GLN
1	A	577	GLN
1	A	599	GLN
1	A	614	HIS
1	B	58	GLN
1	B	79	GLN
1	B	111	ASN
1	B	125	ASN
1	B	129	HIS
1	B	148	ASN
1	B	175	GLN
1	B	187	HIS
1	B	211	GLN
1	B	390	ASN
1	B	423	GLN
1	B	430	GLN
1	B	467	HIS
1	B	472	GLN
1	B	564	GLN
1	B	577	GLN
1	B	583	HIS
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	194	ASN
1	C	201	HIS
1	C	241	ASN
1	C	390	ASN
1	C	423	GLN
1	C	467	HIS

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Mol	Chain	Res	Type
1	C	472	GLN
1	C	494	HIS
1	C	558	GLN
1	C	577	GLN
1	C	599	GLN
1	D	58	GLN
1	D	78	HIS
1	D	79	GLN
1	D	111	ASN
1	D	125	ASN
1	D	148	ASN
1	D	175	GLN
1	D	201	HIS
1	D	232	GLN
1	D	241	ASN
1	D	419	ASN
1	D	423	GLN
1	D	472	GLN
1	D	542	ASN
1	D	558	GLN
1	D	577	GLN
1	D	599	GLN
1	E	58	GLN
1	E	61	HIS
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	214	ASN
1	E	232	GLN
1	E	423	GLN
1	E	467	HIS
1	E	472	GLN
1	E	542	ASN
1	E	558	GLN
1	E	577	GLN
1	F	58	GLN
1	F	61	HIS
1	F	78	HIS
1	F	79	GLN

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Mol	Chain	Res	Type
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
1	F	390	ASN
1	F	400	GLN
1	F	423	GLN
1	F	472	GLN
1	F	558	GLN
1	F	577	GLN
1	F	599	GLN
1	G	58	GLN
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	201	HIS
1	G	214	ASN
1	G	241	ASN
1	G	423	GLN
1	G	470	ASN
1	G	472	GLN
1	G	530	ASN
1	G	542	ASN
1	G	558	GLN
1	G	577	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	187	HIS
1	H	201	HIS
1	H	214	ASN

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Mol	Chain	Res	Type
1	H	423	GLN
1	H	467	HIS
1	H	472	GLN
1	H	558	GLN
1	H	577	GLN
1	H	583	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	E	701	1	0,1,1	-	-	-		
3	CUK	E	702	1	0,6,6	-	-	-		
8	N2O	D	640	-	0,2,2	-	-	0,1,1	-	-
7	IMD	D	639	-	5,5,5	0.68	0	5,5,5	0.36	0
3	CUK	D	702	1	0,6,6	-	-	-		
2	CUA	G	701	1	0,1,1	-	-	-		
8	N2O	H	640	-	0,2,2	-	-	0,1,1	-	-
3	CUK	C	702	1	0,6,6	-	-	-		

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	-	-	-		
3	CUK	F	702	1	0,6,6	-	-	-		
2	CUA	C	701	1	0,1,1	-	-	-		
2	CUA	B	701	1	0,1,1	-	-	-		
2	CUA	H	701	1	0,1,1	-	-	-		
7	IMD	G	639	-	5,5,5	0.66	0	5,5,5	0.40	0
7	IMD	E	639	-	5,5,5	0.66	0	5,5,5	0.35	0
3	CUK	A	702	1	0,6,6	-	-	-		
2	CUA	D	701	1	0,1,1	-	-	-		
7	IMD	F	639	-	5,5,5	0.61	0	5,5,5	0.57	0
7	IMD	H	639	-	5,5,5	0.80	0	5,5,5	0.06	0
3	CUK	H	702	1	0,6,6	-	-	-		
7	IMD	E	640	-	5,5,5	0.72	0	5,5,5	0.46	0
2	CUA	F	701	1	0,1,1	-	-	-		
3	CUK	B	702	1	0,6,6	-	-	-		
3	CUK	G	702	1	0,6,6	-	-	-		

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

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	640	N2O	1	0
7	D	639	IMD	2	0
3	C	702	CUK	1	0
7	G	639	IMD	2	0
7	E	639	IMD	1	0
7	F	639	IMD	2	0
7	H	639	IMD	4	0
3	H	702	CUK	1	0
7	E	640	IMD	3	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, 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%)	0.38	9 (1%) 72 73	12, 30, 52, 61	1 (0%)
1	B	581/638 (91%)	0.29	9 (1%) 72 73	10, 27, 46, 57	3 (0%)
1	C	581/638 (91%)	-0.36	1 (0%) 91 92	7, 14, 28, 39	3 (0%)
1	D	588/638 (92%)	-0.22	0 100 100	7, 18, 32, 43	2 (0%)
1	E	581/638 (91%)	-0.45	1 (0%) 91 92	7, 11, 23, 31	1 (0%)
1	F	581/638 (91%)	-0.41	1 (0%) 91 92	6, 12, 26, 35	3 (0%)
1	G	585/638 (91%)	-0.17	5 (0%) 81 82	8, 17, 39, 53	1 (0%)
1	H	581/638 (91%)	-0.29	3 (0%) 87 88	6, 15, 30, 38	3 (0%)
All	All	4659/5104 (91%)	-0.15	29 (0%) 85 87	6, 18, 40, 61	17 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	638	ALA	3.4
1	G	309	ASP	3.0
1	A	580	ASP	2.9
1	H	523	MET	2.9
1	B	551	MET	2.8
1	A	293	ILE	2.8
1	A	458	ASP	2.7
1	B	60	ILE	2.6
1	G	262	PHE	2.5
1	A	207	VAL	2.5
1	B	537	VAL	2.4
1	G	310	GLY	2.4
1	B	302	VAL	2.3
1	B	638	ALA	2.2
1	B	289	ALA	2.2
1	C	458	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	314	LYS	2.2
1	E	59	LYS	2.2
1	A	282	ALA	2.2
1	B	575	ILE	2.1
1	F	308	LYS	2.1
1	G	580	ASP	2.1
1	A	310	GLY	2.1
1	B	493	PRO	2.1
1	G	497	ILE	2.0
1	H	61	HIS	2.0
1	A	303	LEU	2.0
1	B	297	ASP	2.0
1	H	119	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 [i](#)

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($\text{\AA}^2$)	Q<0.9
6	K	H	705	1/1	0.69	0.16	56,56,56,56	0
6	K	A	705	1/1	0.72	0.14	56,56,56,56	0
6	K	E	705	1/1	0.77	0.14	55,55,55,55	0
6	K	G	705	1/1	0.79	0.14	57,57,57,57	0
6	K	B	705	1/1	0.83	0.14	62,62,62,62	0
7	IMD	G	639	5/5	0.84	0.16	27,28,28,28	0
6	K	C	705	1/1	0.85	0.10	40,40,40,40	0
3	CUK	B	702	6/6	0.89	0.14	51,53,55,57	6
7	IMD	F	639	5/5	0.91	0.10	32,33,33,34	0
6	K	F	705	1/1	0.91	0.09	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	N2O	H	640	3/3	0.92	0.20	51,51,51,52	0
7	IMD	H	639	5/5	0.93	0.09	11,13,14,14	0
8	N2O	D	640	3/3	0.93	0.25	43,43,44,45	0
3	CUK	H	702	6/6	0.93	0.13	32,36,39,41	6
3	CUK	G	702	6/6	0.94	0.10	33,38,40,42	6
2	CUA	A	701	2/2	0.94	0.05	30,30,30,33	0
5	CL	B	704	1/1	0.94	0.17	45,45,45,45	0
6	K	D	705	1/1	0.94	0.09	42,42,42,42	0
7	IMD	D	639	5/5	0.94	0.13	27,27,28,28	0
5	CL	A	704	1/1	0.95	0.15	39,39,39,39	0
3	CUK	A	702	6/6	0.95	0.10	42,45,47,47	6
7	IMD	E	639	5/5	0.95	0.07	26,27,28,28	0
2	CUA	F	701	2/2	0.95	0.04	18,18,18,21	0
3	CUK	C	702	6/6	0.96	0.11	27,31,34,34	6
3	CUK	E	702	6/6	0.96	0.09	27,32,35,36	6
4	CA	A	703	1/1	0.96	0.05	37,37,37,37	0
4	CA	H	703	1/1	0.96	0.03	9,9,9,9	0
7	IMD	E	640	5/5	0.96	0.08	12,12,14,14	0
4	CA	B	703	1/1	0.97	0.03	23,23,23,23	0
3	CUK	F	702	6/6	0.97	0.07	22,27,28,29	5
2	CUA	C	701	2/2	0.97	0.03	21,21,21,25	0
2	CUA	G	701	2/2	0.97	0.03	15,15,15,18	0
2	CUA	D	701	2/2	0.97	0.03	17,17,17,18	0
4	CA	D	703	1/1	0.98	0.05	19,19,19,19	0
4	CA	E	703	1/1	0.98	0.02	10,10,10,10	0
4	CA	G	703	1/1	0.98	0.03	31,31,31,31	0
2	CUA	H	701	2/2	0.98	0.03	29,29,29,31	0
2	CUA	B	701	2/2	0.98	0.03	37,37,37,38	0
3	CUK	D	702	6/6	0.98	0.07	27,32,32,35	6
5	CL	C	704	1/1	0.98	0.10	24,24,24,24	0
5	CL	H	704	1/1	0.98	0.09	27,27,27,27	0
5	CL	D	704	1/1	0.99	0.12	25,25,25,25	0
5	CL	E	704	1/1	0.99	0.06	20,20,20,20	0
5	CL	F	704	1/1	0.99	0.06	17,17,17,17	0
5	CL	G	704	1/1	0.99	0.05	26,26,26,26	0
4	CA	F	703	1/1	0.99	0.02	13,13,13,13	0
2	CUA	E	701	2/2	0.99	0.02	14,14,14,17	0
4	CA	C	703	1/1	0.99	0.02	11,11,11,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.