Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:00 PM GMT

PDB ID	:	3SBR
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

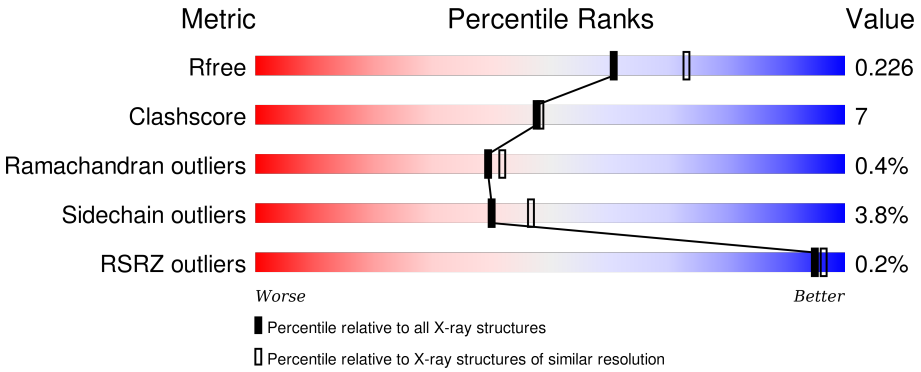
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	% 77% 13% • 9%
1	B	638	75% 15% • 9%
1	C	638	78% 11% • 9%
1	D	638	79% 11% • 8%
1	E	638	76% 13% • 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	638	79% 11% • 9%
1	G	638	% 78% 12% • 8%
1	H	638	75% 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
5	CL	A	704	-	-	X	-
7	IMD	D	639	-	-	-	X
7	IMD	E	640	-	-	-	X
7	IMD	F	639	-	-	-	X
7	IMD	H	639	-	-	X	-
8	N2O	D	640	-	-	-	X
8	N2O	H	640	-	-	-	X

2 Entry composition (i)

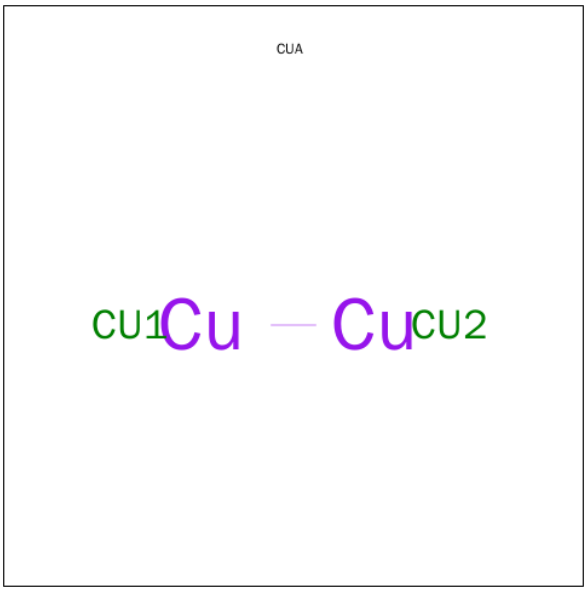
There are 9 unique types of molecules in this entry. The entry contains 39507 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

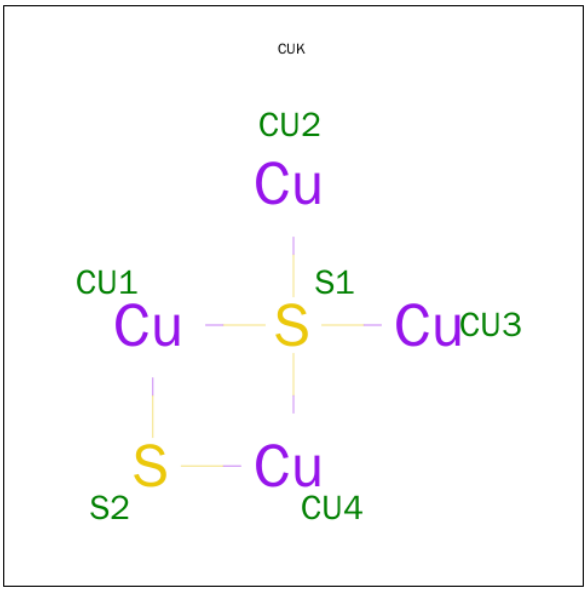
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	1	0
			4573	2891	788	862	32			
1	B	581	Total	C	N	O	S	0	3	0
			4592	2902	792	866	32			
1	C	581	Total	C	N	O	S	0	3	0
			4590	2900	790	868	32			
1	D	588	Total	C	N	O	S	0	2	0
			4636	2929	799	876	32			
1	E	581	Total	C	N	O	S	0	1	0
			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 (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 2 2	0	0
2	B	1	Total Cu 2 2	0	0
2	C	1	Total Cu 2 2	0	0
2	D	1	Total Cu 2 2	0	0
2	E	1	Total Cu 2 2	0	0
2	F	1	Total Cu 2 2	0	0
2	G	1	Total Cu 2 2	0	0
2	H	1	Total Cu 2 2	0	0

- Molecule 3 is [4CU:2S] CLUSTER (three-letter code: CUK) (formula: Cu_4S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu S 6 4 2	0	0
3	B	1	Total Cu S 6 4 2	0	0
3	C	1	Total Cu S 6 4 2	0	0
3	D	1	Total Cu S 6 4 2	0	0
3	E	1	Total Cu S 6 4 2	0	0
3	F	1	Total Cu S 6 4 2	0	0
3	G	1	Total Cu S 6 4 2	0	0
3	H	1	Total Cu S 6 4 2	0	0

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

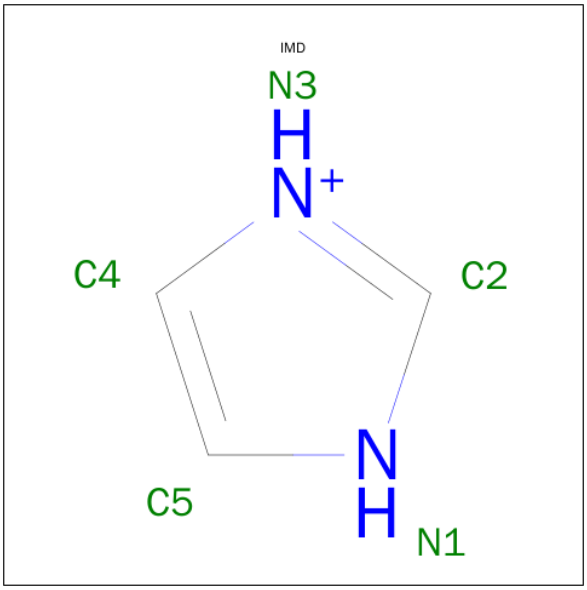
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	E	1	Total K 1 1	0	0
6	H	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0

Continued on next page...

Continued from previous page...

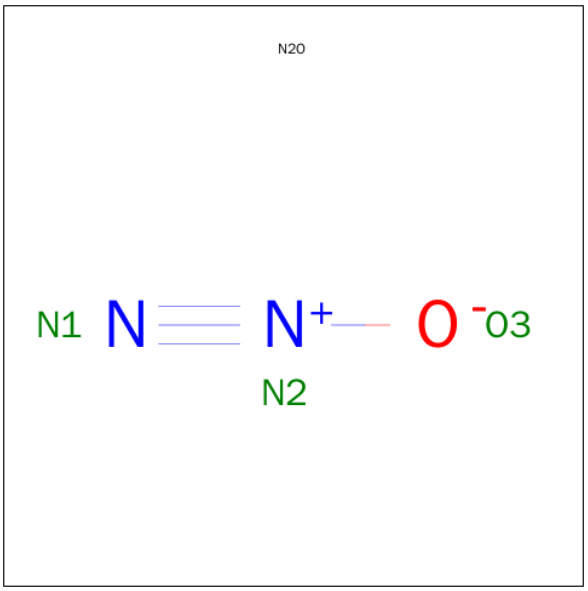
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0
6	F	1	Total K 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C N 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 (three-letter code: N2O) (formula: N_2O).



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

- Molecule 9 is water.

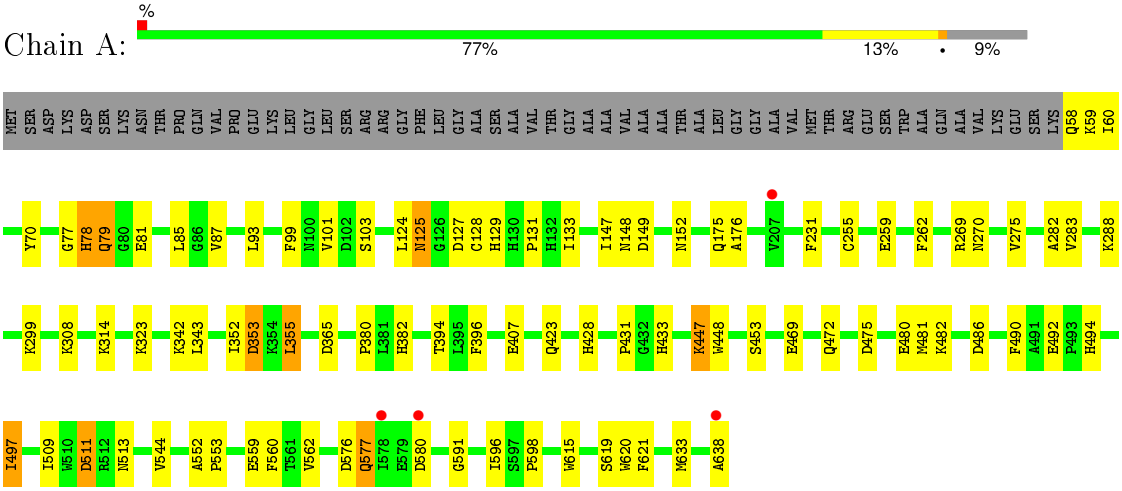
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	207	Total O 207 207	0	0
9	B	183	Total O 183 183	0	0
9	C	367	Total O 367 367	0	0
9	D	365	Total O 365 365	0	0
9	E	393	Total O 393 393	0	0
9	F	411	Total O 411 411	0	0
9	G	349	Total O 349 349	0	0
9	H	353	Total O 353 353	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

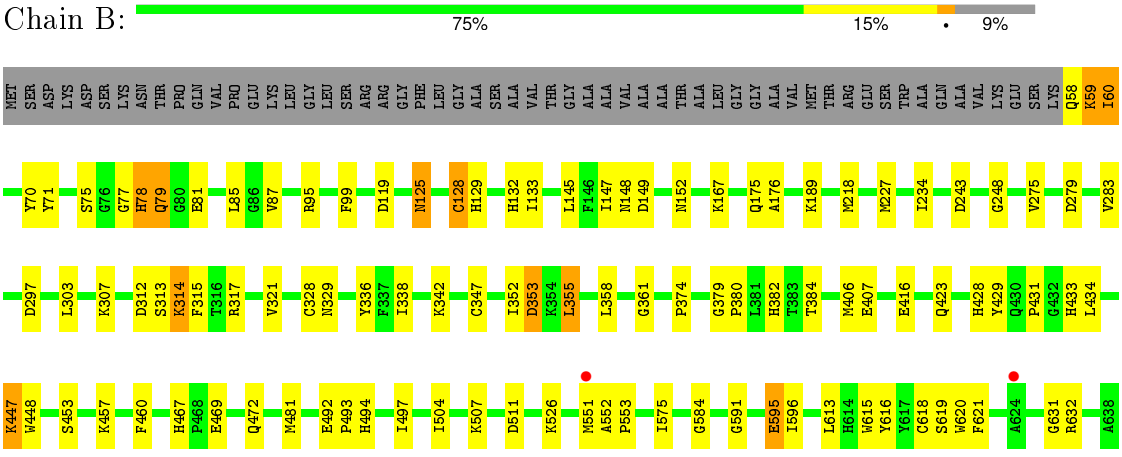
- Molecule 1: Nitrous-oxide reductase

Chain A:



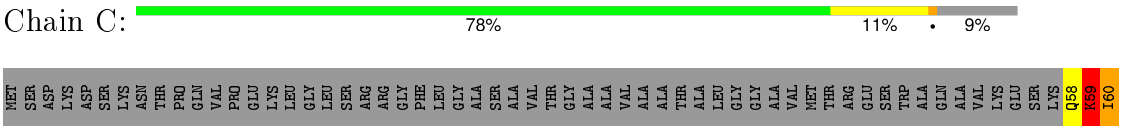
- Molecule 1: Nitrous-oxide reductase

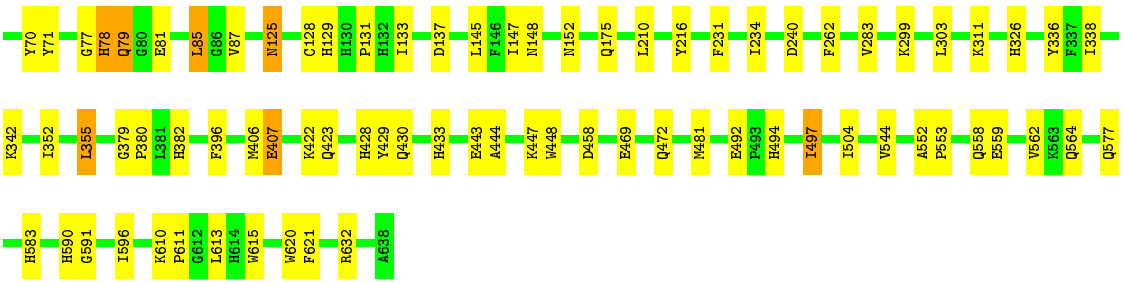
Chain B:



- Molecule 1: Nitrous-oxide reductase

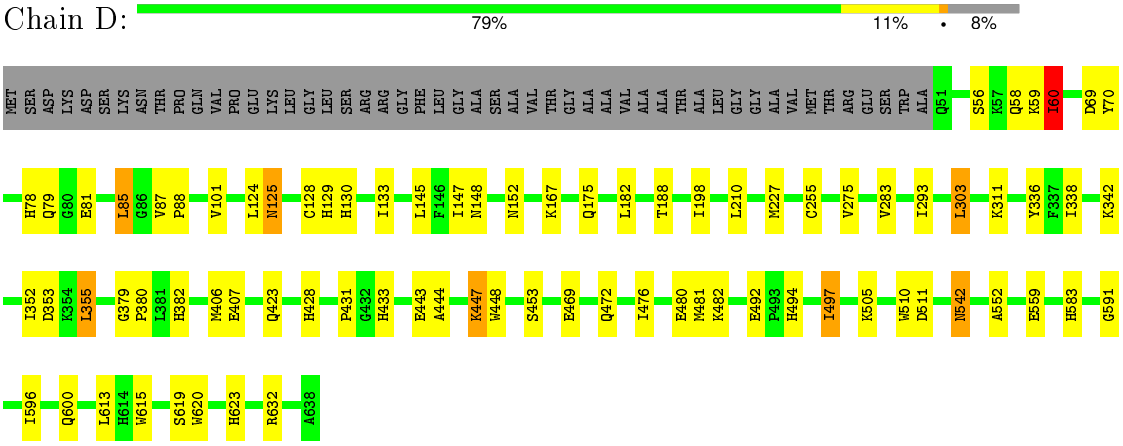
Chain C:





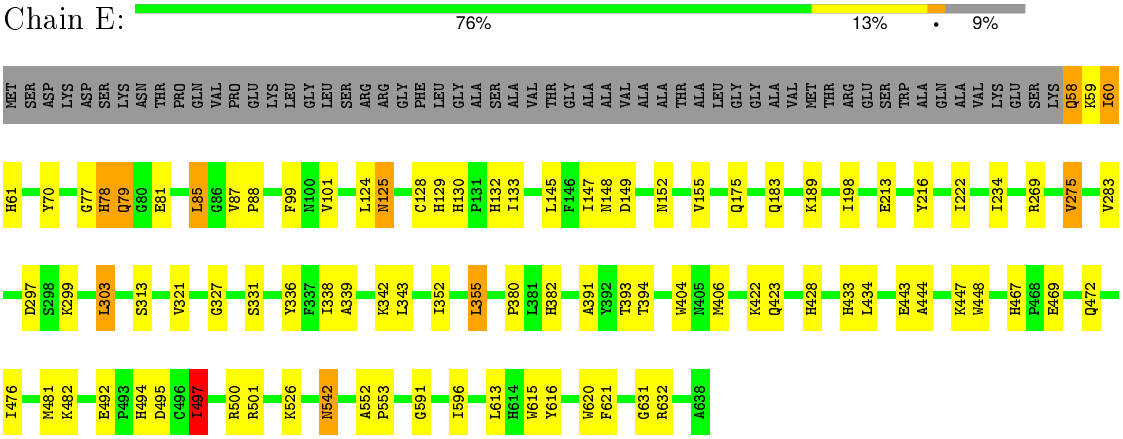
• Molecule 1: Nitrous-oxide reductase

Chain D:



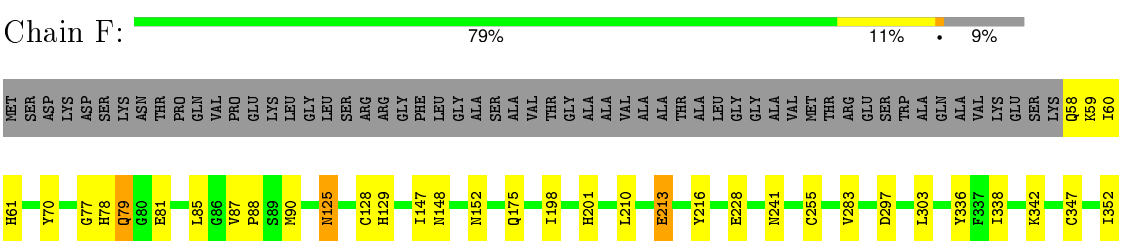
• Molecule 1: Nitrous-oxide reductase

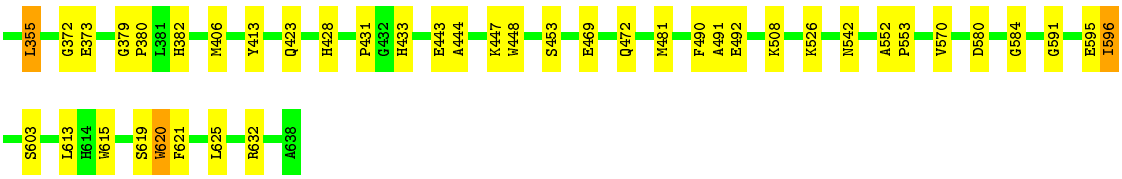
Chain E:



• Molecule 1: Nitrous-oxide reductase

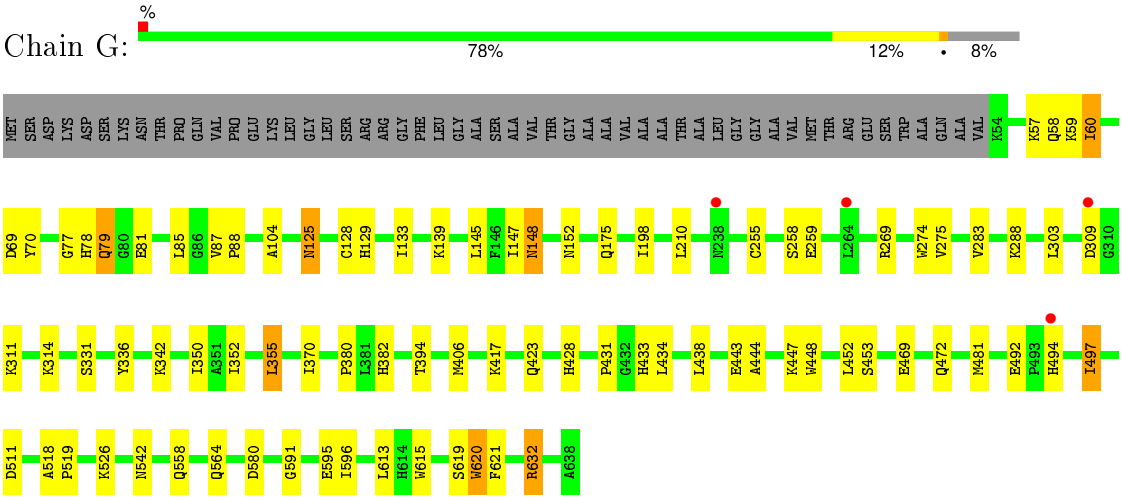
Chain F:





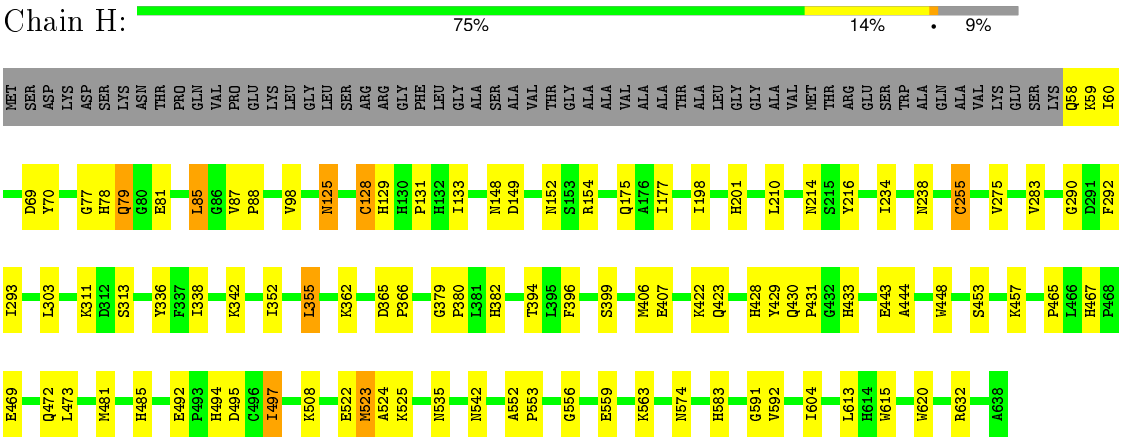
- Molecule 1: Nitrous-oxide reductase

Chain G:



- Molecule 1: Nitrous-oxide reductase

Chain H:



4 Data and refinement statistics (i)

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 95.06 – 2.24	Depositor EDS
% Data completeness (in resolution range)	93.3 (95.00-2.24) 82.3 (95.06-2.24)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.29%)	DCC
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.1	EDS
Estimated twinning fraction	0.012 for -h,k,-k-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 205171 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N2O, IMD, CL, K, CUA, CUK, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.46	0/4685	0.61	1/6345 (0.0%)
1	B	0.48	0/4705	0.61	0/6372
1	C	0.57	0/4702	0.65	1/6368 (0.0%)
1	D	0.53	0/4748	0.66	1/6428 (0.0%)
1	E	0.59	0/4687	0.69	3/6348 (0.0%)
1	F	0.57	0/4705	0.66	1/6372 (0.0%)
1	G	0.54	0/4718	0.66	2/6387 (0.0%)
1	H	0.57	0/4702	0.67	1/6368 (0.0%)
All	All	0.54	0/37652	0.65	10/50988 (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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	85	LEU	CA-CB-CG	6.78	130.90	115.30
1	E	85	LEU	CA-CB-CG	6.28	129.74	115.30
1	E	303	LEU	CA-CB-CG	-6.26	100.89	115.30
1	G	632	ARG	NE-CZ-NH2	-6.16	117.22	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	497	ILE	CB-CA-C	-5.58	100.44	111.60
1	A	85	LEU	CA-CB-CG	5.56	128.08	115.30
1	D	85	LEU	CA-CB-CG	5.44	127.81	115.30
1	G	632	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	F	85	LEU	CA-CB-CG	5.16	127.17	115.30
1	H	85	LEU	CA-CB-CG	5.02	126.86	115.30

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 (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	59	0
1	B	4592	0	4452	84	0
1	C	4590	0	4449	70	0
1	D	4636	0	4505	64	0
1	E	4575	0	4440	86	0
1	F	4593	0	4450	66	0
1	G	4606	0	4478	71	0
1	H	4590	0	4449	81	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	539	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (539) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:338:ILE:HD11	1:H:406:MET:CE	1.80	1.10
9:D:2328:HOH:O	1:E:542:ASN:HB3	1.58	1.03
1:F:338:ILE:HD11	1:F:406:MET:HE3	1.40	1.01
1:E:336:TYR:HD2	1:E:406:MET:HE1	1.26	0.97
1:F:336:TYR:HD2	1:F:406:MET:HE1	1.31	0.96
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: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: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:H:338:ILE:HD11	1:H:406:MET:HE3	1.59	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:H:338:ILE:HD11	1:H:406:MET:HE2	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:ILE:HD11	1:E:406:MET:HE3	1.60	0.83
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:336:TYR:CD2	1:F:406:MET:HE1	2.13	0.83
1:F:469:GLU:HG3	1:F:492:GLU:HA	1.61	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:H:423:GLN:HE22	1:H:481:MET:H	1.29	0.81
1:C:338:ILE:HD11	1:C:406:MET:HE3	1.64	0.80
1:H:338:ILE:CD1	1:H:406:MET:CE	2.60	0.80
1:G:129:HIS:H	1:G:148:ASN:HD21	1.29	0.80
1:E:336:TYR:CD2	1:E:406:MET:HE1	2.15	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: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:E:125:ASN:HD21	1:F:591:GLY:HA2	1.46	0.78
1:A:352:ILE:HA	1:A:355:LEU:HD22	1.65	0.78
1:G:331:SER:HB3	1:G:406:MET:HE3	1.66	0.78
1:H:338:ILE:CD1	1:H:406:MET:HE3	2.13	0.78
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:C:382:HIS:CE1	1:C:433:HIS:CE1	2.72	0.77
1:E:338:ILE:HD11	1:E:406:MET:CE	2.15	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:B:338:ILE:HD11	1:B:406:MET:HE3	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:E:59:LYS:NZ	1:E:448:TRP:HE1	1.86	0.73
1:C:137:ASP:HB3	9:C:1790:HOH:O	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:LYS:HE2	1:H:88:PRO:HG3	1.70	0.73
1:H:59:LYS:HZ3	1:H:448:TRP:HE1	1.37	0.72
1:H:382:HIS:NE2	1:H:433:HIS:CD2	2.57	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:C:336:TYR:HD2	1:C:406:MET:HE1	1.55	0.72
1:D:352:ILE:HA	1:D:355:LEU:HD22	1.70	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:D:336:TYR:HD2	1:D:406:MET:CE	2.03	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: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:B:336:TYR:HD2	1:B:406:MET:HE1	1.53	0.71
1:C:613:LEU:HD11	1:C:632:ARG:HB3	1.72	0.71
1:C:283:VAL:HG13	1:C:303:LEU:CD1	2.21	0.71
1:D:428:HIS:H	1:D:472:GLN:HE22	1.36	0.70
1:B:338:ILE:HD11	1:B:406:MET:CE	2.21	0.70
1:F:198:ILE:H	7:F:639:IMD:H2	1.57	0.70
1:C:338:ILE:HD11	1:C:406:MET:CE	2.22	0.69
1:E:70:TYR:HB2	1:E:87:VAL:HB	1.75	0.69
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
1:C:125:ASN:HD21	1:D:591:GLY:HA2	1.60	0.67
1:B:382[A]:HIS:CE1	1:B:433:HIS:NE2	2.62	0.67
1:C:552:ALA:HB2	1:C:583:HIS:HE1	1.60	0.67
1:H:382:HIS:CE1	1:H:433:HIS:NE2	2.63	0.66
1:D:542:ASN:HB3	9:D:654:HOH:O	1.94	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: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:H:59:LYS:NZ	1:H:448:TRP:HE1	1.92	0.65
1:A:70:TYR:HB2	1:A:87:VAL:HB	1.79	0.65
1:D:336:TYR:HD2	1:D:406:MET:HE1	1.62	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:E:59:LYS:CE	1:E:88:PRO:HG3	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:338:ILE:CD1	1:F:406:MET:HE3	2.24	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: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: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:E:338:ILE:CD1	1:E:406:MET:HE3	2.31	0.61
1:H:128:CYS:HB3	1:H:148:ASN:O	2.00	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:E:59:LYS:O	1:E:60:ILE:HG23	2.01	0.60
1:A:469:GLU:HG3	1:A:492:GLU:HA	1.82	0.60
1:C:129:HIS:H	1:C:148:ASN:ND2	1.98	0.60
1:B:382[B]:HIS:HD2	1:B:434:LEU:HD23	1.67	0.60
1:D:70:TYR:HB2	1:D:87:VAL:HB	1.84	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:G:336:TYR:CD2	1:G:406:MET:HE2	2.37	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:B:336:TYR:CD2	1:B:406:MET:HE1	2.38	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:429:TYR:CD1	1:B:457:LYS:HD2	2.38	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:F:148:ASN:HD22	1:F:148:ASN:H	1.51	0.57
1:E:61:HIS:HB3	9:F:1215:HOH:O	2.05	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:G:331:SER:HB3	1:G:406:MET:CE	2.35	0.56
1:C:59:LYS:NZ	1:C:448:TRP:HE1	2.03	0.56
1:A:99:PHE:CE2	1:A:149:ASP:HB2	2.39	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: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: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:D:336:TYR:CD2	1:D:406:MET:CE	2.89	0.55
1:F:336:TYR:CD2	1:F:406:MET:CE	2.87	0.55
1:F:428:HIS:H	1:F:472:GLN:NE2	2.03	0.55
1:B:79:GLN:HE22	1:B:81:GLU:CG	2.19	0.55
1:H:338:ILE:CD1	1:H:406:MET:HE2	2.34	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:C:423:GLN:HE22	1:C:481:MET:N	1.95	0.55
1:B:379:GLY:N	1:B:380:PRO:HD3	2.22	0.55
1:H:423:GLN:HE22	1:H:481:MET:N	2.03	0.55
1:G:619:SER:O	1:H:78:HIS:CE1	2.60	0.55
1:A:544:VAL:HG21	1:A:562:VAL:HG12	1.88	0.55
1:H:428:HIS:H	1:H:472:GLN:NE2	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:HIS:CE1	1:B:619:SER:O	2.61	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:C:591:GLY:HA2	1:D:125:ASN:ND2	2.23	0.54
1:H:198:ILE:H	7:H:639:IMD:HN3	1.56	0.54
1:F:90:MET:HG3	9:F:2183:HOH:O	2.07	0.54
1:H:542:ASN:HB3	9:H:1267:HOH:O	2.07	0.54
1:F:632:ARG:HD3	9:F:1451: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
1:G:564:GLN:HG2	9:G:2944:HOH:O	2.07	0.53
1:F:447:LYS:HE2	9:F:2850:HOH:O	2.08	0.53
1:E:613:LEU:HD11	1:E:632:ARG:HG2	1.89	0.53
1:G:336:TYR:CD2	1:G:406:MET:CE	2.88	0.53
1:G:129:HIS:N	1:G:148:ASN:HD21	2.04	0.53
1:C:336:TYR:HD2	1:C:406:MET:CE	2.22	0.53
1:C:231:PHE:CE1	1:C:283:VAL:HG11	2.43	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:G:352:ILE:HA	1:G:355:LEU:HD22	1.91	0.52
1:C:145:LEU:HD11	1:C:497:ILE:HD11	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: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:B:77:GLY:HA2	1:B:128:CYS:O	2.10	0.52
1:A:511:ASP:HB3	1:A:513:ASN:OD1	2.10	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:D:542:ASN:C	1:D:542:ASN:HD22	2.14	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:LYS:HE2	1:D:88:PRO:HG3	1.92	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:G:258:SER:HB2	1:G:274:TRP:CZ3	2.45	0.51
1:E:99:PHE:CE2	1:E:149:ASP:HB2	2.45	0.51
1:D:428:HIS:H	1:D:472:GLN:NE2	2.07	0.51
1:E:382:HIS:CD2	1:E:433:HIS:CD2	2.99	0.51
1:C:336:TYR:CD2	1:C:406:MET:HE1	2.41	0.50
1:G:198:ILE:H	7:G:639:IMD:C4	2.22	0.50
1:C:428:HIS:H	1:C:472:GLN:HE22	1.58	0.50
1:C:615:TRP:H	1:D:175:GLN:HE22	1.57	0.50
1:A:282:ALA:HB1	1:A:314:LYS:HD2	1.93	0.50
1:D:129:HIS:CE1	1:D:494:HIS:CE1	2.98	0.50
1:D:336:TYR:CD2	1:D:406:MET:HE2	2.46	0.50
1:B:382[A]:HIS:NE2	1:B:433:HIS:NE2	2.58	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:A:129:HIS:CE1	1:A:494:HIS:CE1	2.99	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: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:F:79:GLN:HE22	1:F:81:GLU:CG	2.25	0.50
1:C:59:LYS:HZ3	1:C:448:TRP:HE1	1.58	0.49
1:E:382:HIS:CE1	5:E:704:CL:CL	3.03	0.49
1:C:615:TRP:HD1	1:D:175:GLN:NE2	2.10	0.49
1:E:467:HIS:HB2	1:F:580:ASP:OD1	2.12	0.49
1:G:283:VAL:CG1	1:G:303:LEU:HD13	2.35	0.49
1:E:59:LYS:HZ3	1:E:448:TRP:HE1	1.56	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:D:59:LYS:HZ3	1:D:448:TRP:HE1	1.60	0.49
1:H:429:TYR:CD2	1:H:457:LYS:HD2	2.48	0.49
1:F:423:GLN:NE2	1:F:481:MET:H	2.01	0.48
1:E:125:ASN:ND2	1:E:152:ASN:HD21	2.11	0.48
1:H:58:GLN:HG2	1:H:59:LYS:HD3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ILE:HG22	1:A:598:PRO:HB2	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:382:HIS:HB3	9:F:2403:HOH:O	2.12	0.48
1:F:128:CYS:HB2	1:F:147:ILE:CD1	2.43	0.48
1:C:433:HIS:HB2	1:C:494:HIS:O	2.14	0.48
1:F:129:HIS:H	1:F:148:ASN:ND2	2.06	0.48
1:E:155:VAL:HG21	1:E:222:ILE:CD1	2.44	0.48
1:H:382:HIS:CD2	1:H:433:HIS:CD2	3.01	0.48
1:B:125:ASN:HD21	1:B:152:ASN:HD21	1.61	0.48
1:F:431:PRO:HA	1:F:453:SER:HA	1.95	0.48
1:B:307:LYS:HG2	1:B:312:ASP:HA	1.95	0.48
1:B:613:LEU:HD11	1:B:632:ARG:HB3	1.94	0.48
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:128:CYS:HB3	1:F:148:ASN:O	2.13	0.48
1:F:125:ASN:ND2	1:F:152:ASN:HD21	2.12	0.48
1:F:490:PHE:CD2	1:F:491:ALA:HB2	2.49	0.48
1:C:336:TYR:CD2	1:C:406:MET:CE	2.97	0.48
1:E:433:HIS:HB2	1:E:494:HIS:O	2.14	0.48
1:G:133:ILE:HG13	1:G:497:ILE:CD1	2.44	0.48
1:F:213[A]:GLU:HG3	1:F:213[A]:GLU:O	2.13	0.48
1:A:619:SER:O	1:B:78:HIS:CE1	2.67	0.48
1:C:262:PHE:HB2	1:D:632:ARG:HD2	1.96	0.47
1:C:338:ILE:CD1	1:C:406:MET:HE3	2.40	0.47
1:D:510:TRP:CD1	1:D:600:GLN:HB2	2.50	0.47
1:D:431:PRO:HA	1:D:453:SER:HA	1.97	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:C:396:PHE:CE1	1:C:430:GLN:HB3	2.50	0.47
1:A:79:GLN:HE22	1:A:81:GLU:CG	2.27	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:D:552:ALA:HB2	1:D:583:HIS:HE1	1.80	0.47
1:H:469:GLU:CG	1:H:492:GLU:HA	2.33	0.47
1:F:128:CYS:HB2	1:F:147:ILE:HD11	1.97	0.47
1:D:559:GLU:HA	1:D:632:ARG:O	2.15	0.47
1:A:78:HIS:HA	1:A:127:ASP:HA	1.97	0.47
1:C:77:GLY:HA2	1:C:128:CYS:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:HIS:CE1	1:E:433:HIS:CE1	3.03	0.47
1:B:59:LYS:NZ	1:B:448:TRP:HE1	2.11	0.47
1:A:323:LYS:HG2	1:A:343:LEU:HB2	1.96	0.47
1:B:243:ASP:HB2	1:B:328:CYS:O	2.15	0.47
1:A:58:GLN:HE22	1:A:447:LYS:HG2	1.79	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:G:431:PRO:HA	1:G:453:SER:HA	1.97	0.47
1:F:595:GLU:HB2	1:F:620:TRP:CZ3	2.50	0.47
1:D:59:LYS:NZ	1:D:448:TRP:HE1	2.13	0.47
1:A:314:LYS:HB2	9:A:1084:HOH:O	2.15	0.47
1:A:59:LYS:NZ	1:A:448:TRP:HE1	2.13	0.47
1:B:353:ASP:HB2	9:B:2008:HOH:O	2.14	0.47
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:H:396:PHE:CE1	1:H:430:GLN:HB3	2.49	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:433:HIS:HB2	1:H:494:HIS:O	2.15	0.46
1:F:595:GLU:HG2	1:F:596:ILE:N	2.29	0.46
1:C:590:HIS:CE1	1:C:610:LYS:HE2	2.50	0.46
1:H:380:PRO:HA	1:H:394:THR:O	2.15	0.46
1:B:75:SER:O	1:B:493:PRO:HB3	2.16	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:C:148:ASN:H	1:C:148:ASN:HD22	1.64	0.46
1:B:128:CYS:HB2	1:B:147:ILE:HD11	1.97	0.46
1:F:372:GLY:HA2	1:F:413:TYR:HB2	1.98	0.46
1:D:148:ASN:H	1:D:148:ASN:HD22	1.63	0.46
1:B:429:TYR:CE1	1:B:457:LYS:HD2	2.50	0.46
1:B:347:CYS:O	1:B:374:PRO:HD2	2.15	0.46
1:E:336:TYR:CD2	1:E:406:MET:HE2	2.51	0.46
1:E:469:GLU:CG	1:E:492:GLU:HA	2.38	0.46
1:G:350:ILE:HG12	1:G:370:ILE:HD13	1.97	0.46
1:C:125:ASN:HD21	1:C:152:ASN:HD21	1.64	0.46
1:F:443:GLU:O	1:F:444:ALA:C	2.54	0.46
1:G:452:LEU:HD22	1:G:494:HIS:O	2.16	0.46
1:E:129:HIS:N	1:E:148:ASN:HD21	2.11	0.46
1:A:129:HIS:H	1:A:148:ASN:ND2	2.10	0.46
1:F:59:LYS:HE2	1:F:88:PRO:HG3	1.98	0.46
1:A:560:PHE:CE2	1:A:633:MET:HG3	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:HIS:H	1:E:148:ASN:ND2	2.14	0.46
1:A:577:GLN:HB3	1:A:577:GLN:HE21	1.56	0.46
1:H:433:HIS:HD2	3:H:702:CUK:S2	2.39	0.46
1:B:148:ASN:HD22	1:B:148:ASN:H	1.64	0.46
1:G:59:LYS:HZ1	1:G:448:TRP:HE1	1.64	0.46
1:D:125:ASN:HD22	1:D:125:ASN:H	1.64	0.45
1:E:338:ILE:HD11	1:E:406:MET:HE2	1.97	0.45
1:E:59:LYS:HZ1	1:E:448:TRP:HE1	1.59	0.45
1:C:145:LEU:CD1	1:C:497:ILE:HD11	2.45	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:E:331:SER:HB3	1:E:406:MET:HE3	1.98	0.45
1:D:128:CYS:HB3	1:D:148:ASN:O	2.16	0.45
1:C:443:GLU:O	1:C:444:ALA:C	2.55	0.45
1:G:125:ASN:ND2	1:G:152:ASN:HD21	2.14	0.45
1:A:396:PHE:HA	1:A:431:PRO:HD2	1.97	0.45
1:G:125:ASN:H	1:G:125:ASN:HD22	1.63	0.45
1:E:58:GLN:N	9:E:1461:HOH:O	2.48	0.45
1:H:473:LEU:HB3	1:H:485:HIS:HB3	1.99	0.45
1:D:447:LYS:HE3	9:D:2098:HOH:O	2.16	0.45
1:D:101:VAL:HG21	1:D:124:LEU:HD22	1.98	0.45
1:B:433:HIS:HB2	1:B:494:HIS:O	2.16	0.45
1:B:428:HIS:H	1:B:472:GLN:NE2	2.14	0.45
1:F:148:ASN:ND2	1:F:148:ASN:H	2.15	0.45
1:H:125:ASN:ND2	1:H:152:ASN:HD21	2.14	0.45
1:E:433:HIS:ND1	1:E:495:ASP:CG	2.70	0.45
1:C:422:LYS:HD3	1:C:422:LYS:HA	1.83	0.45
1:A:638:ALA:HA	9:A:1042:HOH:O	2.17	0.44
1:A:615:TRP:H	1:B:175:GLN:HE22	1.66	0.44
1:E:58:GLN:CG	1:E:59:LYS:HD3	2.48	0.44
1:C:70:TYR:HB2	1:C:87:VAL:HB	1.97	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: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:C:216:TYR:CD1	1:C:234:ILE:HG23	2.52	0.44
1:B:275:VAL:HG13	1:B:321:VAL:HG21	1.99	0.44
1:A:101:VAL:HG21	1:A:124:LEU:HD22	1.98	0.44
1:E:327:GLY:O	1:E:339:ALA:HA	2.18	0.44
1:H:148:ASN:H	1:H:148:ASN:HD22	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:615:TRP:H	1:H:175:GLN:NE2	2.15	0.44
1:B:125:ASN:ND2	1:B:152:ASN:HD21	2.14	0.44
1:G:145:LEU:HD12	1:G:497:ILE:HD11	2.00	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:A:133:ILE:HG13	1:A:497:ILE:HD13	2.00	0.44
1:H:552:ALA:HA	1:H:553:PRO:HA	1.81	0.44
1:A:480:GLU:OE1	1:F:526:LYS:HE3	2.17	0.44
1:B:279:ASP:O	1:B:283:VAL:HG23	2.17	0.44
1:C:283:VAL:HG13	1:C:303:LEU:HD13	1.98	0.44
1:A:472:GLN:HG2	1:A:486:ASP:OD1	2.18	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:G:558:GLN:NE2	9:G:695:HOH:O	2.49	0.44
1:B:431:PRO:HA	1:B:453:SER:HA	1.99	0.44
1:B:59:LYS:HB3	1:B:60:ILE:H	1.46	0.43
1:G:59:LYS:CE	1:G:88:PRO:HG3	2.48	0.43
1:F:490:PHE:CE2	1:F:491:ALA:HB2	2.53	0.43
1:C:544:VAL:HG21	1:C:562:VAL:HG12	1.99	0.43
1:F:213[A]:GLU:CG	1:F:213[A]:GLU:O	2.65	0.43
1:G:380:PRO:HA	1:G:394:THR:O	2.18	0.43
1:A:380:PRO:HA	1:A:394:THR:O	2.17	0.43
1:A:103:SER:HB2	1:B:125:ASN:HA	2.00	0.43
1:F:128:CYS:HB2	1:F:147:ILE:HG12	2.00	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:B:595:GLU:HG2	1:B:596:ILE:N	2.34	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:A:128:CYS:HB3	1:A:148:ASN:O	2.18	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:G:497:ILE:HG21	9:G:675:HOH:O	2.17	0.43
1:C:71:TYR:CE1	1:C:504:ILE:HB	2.54	0.43
1:E:382:HIS:CG	9:E:1097:HOH:O	2.72	0.43
1:E:78:HIS:ND1	9:E:1432:HOH:O	2.35	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:H:362:LYS:NZ	9:H:715:HOH:O	2.52	0.43
1:E:616:TYR:CE1	1:E:631:GLY:HA3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:443:GLU:O	1:E:444:ALA:C	2.57	0.42
1:B:303:LEU:HD22	1:B:315:PHE:CZ	2.53	0.42
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:E:275:VAL:CG1	1:E:321:VAL:HG21	2.50	0.42
1:B:338:ILE:HD11	1:B:406:MET:HE2	1.99	0.42
1:H:77:GLY:HA2	1:H:128:CYS:O	2.19	0.42
1:B:329:ASN:HD21	1:B:382[B]:HIS:CE1	2.38	0.42
1:G:259:GLU:HG2	1:G:269:ARG:HB3	2.01	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:B:58:GLN:HE22	1:B:447:LYS:HG2	1.84	0.42
1:E:391:ALA:HB3	1:E:404:TRP:CE2	2.54	0.42
1:H:422:LYS:HA	1:H:422:LYS:HD3	1.82	0.42
1:D:133:ILE:HG13	1:D:497:ILE:CD1	2.49	0.42
1:B:552:ALA:HA	1:B:553:PRO:HA	1.73	0.42
1:H:336:TYR:HD2	1:H:406:MET:HE1	1.84	0.42
1:E:128:CYS:HB2	1:E:147:ILE:HG12	2.02	0.42
1:B:382[B]:HIS:HD2	1:B:434:LEU:H	1.68	0.42
1:C:552:ALA:HA	1:C:553:PRO:HA	1.82	0.42
1:B:613:LEU:CD1	1:B:632:ARG:HB3	2.50	0.42
1:C:469:GLU:CG	1:C:492:GLU:HA	2.34	0.42
1:F:125:ASN:HD21	1:F:152:ASN:HD21	1.68	0.42
1:C:58:GLN:HG2	1:C:59:LYS:HD3	2.02	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:D:130:HIS:H	1:D:148:ASN:ND2	2.17	0.42
7:E:640:IMD:H2	1:F:615:TRP:CZ2	2.54	0.42
1:C:428:HIS:HA	1:C:429:TYR:CG	2.55	0.42
1:D:167:LYS:CB	1:D:227:MET:HG3	2.50	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:H:382:HIS:CE1	5:H:704:CL:CL	3.10	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:ILE:HD11	1:D:406:MET:HE3	2.01	0.41
1:B:79:GLN:HB3	1:B:79:GLN:HE21	1.61	0.41
1:G:175:GLN:NE2	1:H:615:TRP:HD1	2.18	0.41
1:G:104:ALA:O	1:G:620:TRP:HZ3	2.04	0.41
1:C:379:GLY:N	1:C:380:PRO:HD3	2.35	0.41
1:A:58:GLN:HB3	1:A:475:ASP:OD2	2.19	0.41
1:H:290:GLY:HA2	1:H:292:PHE:CE2	2.56	0.41
1:E:552:ALA:HA	1:E:553:PRO:HA	1.84	0.41
1:E:132:HIS:O	1:E:145:LEU:HA	2.20	0.41
1:E:331:SER:HB3	1:E:406:MET:CE	2.50	0.41
1:B:283:VAL:CG1	1:B:303:LEU:HD13	2.40	0.41
1:A:591:GLY:HA2	1:B:125:ASN:ND2	2.33	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:E:382:HIS:CB	9:E:1097:HOH:O	2.56	0.41
1:B:167:LYS:CB	1:B:227:MET:HG3	2.50	0.41
1:A:490:PHE:CD2	1:B:95:ARG:HD2	2.55	0.41
1:E:382:HIS:O	1:E:393:THR:HA	2.21	0.41
1:B:125:ASN:H	1:B:125:ASN:HD22	1.68	0.41
1:E:343:LEU:HD21	1:F:625:LEU:HD21	2.02	0.41
1:H:338:ILE:HD12	1:H:406:MET:HE3	1.99	0.41
1:C:382:HIS:CE1	5:C:704:CL:CL	3.11	0.41
1:H:148:ASN:HB2	1:H:177:ILE:HG22	2.03	0.41
1:C:131:PRO:O	1:C:497:ILE:HG12	2.21	0.41
1:F:552:ALA:HA	1:F:553:PRO:HA	1.86	0.41
1:E:422:LYS:HA	1:E:422:LYS:HD3	1.91	0.41
1:F:241:ASN:ND2	5:F:704:CL:CL	2.91	0.41
1:H:70:TYR:HB2	1:H:87:VAL:HB	2.03	0.41
1:G:309:ASP:C	1:G:311:LYS:H	2.25	0.41
1:D:56:SER:H	1:D:482:LYS:NZ	2.19	0.41
9:E:2589:HOH:O	1:F:61:HIS:HB3	2.21	0.41
1:D:443:GLU:O	1:D:444:ALA:C	2.59	0.41
1:C:128:CYS:HB2	1:C:147:ILE:CD1	2.51	0.41
1:H:433:HIS:ND1	1:H:495:ASP:CG	2.74	0.41
7:E:640:IMD:H2	1:F:615:TRP:CH2	2.56	0.41
1:E:380:PRO:HA	1:E:394:THR:O	2.21	0.41
1:D:182:LEU:HB3	1:D:188:THR:HG23	2.03	0.41
1:D:476:ILE:HG22	1:D:481:MET:HG2	2.01	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:GLY:O	1:B:618:CYS:HA	2.21	0.40
1:H:443:GLU:O	1:H:444:ALA:C	2.58	0.40
1:G:580:ASP:OD1	1:H:467:HIS:HB2	2.21	0.40
1:G:518:ALA:N	1:G:519:PRO:CD	2.84	0.40
1:B:129:HIS:N	1:B:148:ASN:HD21	2.14	0.40
1:A:231:PHE:CE1	1:A:283:VAL:HG11	2.57	0.40
1:G:433:HIS:HB2	1:G:494:HIS:O	2.21	0.40
1:G:336:TYR:HA	1:G:350:ILE:O	2.22	0.40
1:B:248:GLY:HA2	9:B:2425:HOH:O	2.21	0.40
1:B:132:HIS:O	1:B:145:LEU:HA	2.21	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:C:133:ILE:HG13	1:C:497:ILE:CD1	2.51	0.40
1:A:58:GLN:HG2	1:A:59:LYS:HB2	2.04	0.40
1:E:500:ARG:O	1:E:501:ARG:C	2.59	0.40
1:B:218:MET:HG2	1:B:234:ILE:HA	2.04	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%)	26	25
1	B	582/638 (91%)	554 (95%)	24 (4%)	4 (1%)	26	25
1	C	582/638 (91%)	560 (96%)	19 (3%)	3 (0%)	34	34
1	D	588/638 (92%)	561 (95%)	25 (4%)	2 (0%)	46	51
1	E	580/638 (91%)	555 (96%)	24 (4%)	1 (0%)	52	60
1	F	582/638 (91%)	552 (95%)	27 (5%)	3 (0%)	34	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	584/638 (92%)	556 (95%)	27 (5%)	1 (0%)	52 60
1	H	582/638 (91%)	557 (96%)	23 (4%)	2 (0%)	46 51
All	All	4660/5104 (91%)	4439 (95%)	201 (4%)	20 (0%)	39 42

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	60	ILE
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 (i)

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%)	475 (96%)	22 (4%)	35 39
1	B	499/537 (93%)	479 (96%)	20 (4%)	38 44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	499/537 (93%)	480 (96%)	19 (4%)	40	47
1	D	504/537 (94%)	485 (96%)	19 (4%)	40	47
1	E	497/537 (93%)	480 (97%)	17 (3%)	44	53
1	F	499/537 (93%)	485 (97%)	14 (3%)	51	61
1	G	501/537 (93%)	481 (96%)	20 (4%)	38	44
1	H	499/537 (93%)	480 (96%)	19 (4%)	40	47
All	All	3995/4296 (93%)	3845 (96%)	150 (4%)	40	47

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ILE
1	A	78	HIS
1	A	79	GLN
1	A	125	ASN
1	A	255	CYS
1	A	270	ASN
1	A	275	VAL
1	A	288	LYS
1	A	353	ASP
1	A	355	LEU
1	A	365	ASP
1	A	407	GLU
1	A	447	LYS
1	A	482	LYS
1	A	497	ILE
1	A	511	ASP
1	A	559	GLU
1	A	576	ASP
1	A	577	GLN
1	A	596	ILE
1	A	620	TRP
1	A	621	PHE
1	B	78	HIS
1	B	79	GLN
1	B	85	LEU
1	B	119	ASP
1	B	125	ASN
1	B	128	CYS
1	B	189	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	447	LYS
1	B	507	LYS
1	B	511	ASP
1	B	526	LYS
1	B	595	GLU
1	B	620	TRP
1	B	621	PHE
1	C	59	LYS
1	C	60	ILE
1	C	78	HIS
1	C	79	GLN
1	C	85	LEU
1	C	125	ASN
1	C	210	LEU
1	C	299	LYS
1	C	311	LYS
1	C	355	LEU
1	C	407	GLU
1	C	447	LYS
1	C	497	ILE
1	C	558	GLN
1	C	559	GLU
1	C	577	GLN
1	C	596	ILE
1	C	620	TRP
1	C	621	PHE
1	D	60	ILE
1	D	78	HIS
1	D	85	LEU
1	D	125	ASN
1	D	210	LEU
1	D	255	CYS
1	D	275	VAL
1	D	293	ILE
1	D	303	LEU
1	D	311	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	353	ASP
1	D	355	LEU
1	D	407	GLU
1	D	447	LYS
1	D	497	ILE
1	D	511	ASP
1	D	542	ASN
1	D	596	ILE
1	D	620	TRP
1	E	60	ILE
1	E	78	HIS
1	E	79	GLN
1	E	85	LEU
1	E	125	ASN
1	E	213	GLU
1	E	275	VAL
1	E	297	ASP
1	E	299	LYS
1	E	313	SER
1	E	355	LEU
1	E	482	LYS
1	E	497	ILE
1	E	542	ASN
1	E	596	ILE
1	E	620	TRP
1	E	621	PHE
1	F	60	ILE
1	F	78	HIS
1	F	79	GLN
1	F	125	ASN
1	F	210	LEU
1	F	228	GLU
1	F	255	CYS
1	F	297	ASP
1	F	355	LEU
1	F	508	LYS
1	F	542	ASN
1	F	596	ILE
1	F	620	TRP
1	F	621	PHE
1	G	57	LYS
1	G	60	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	78	HIS
1	G	79	GLN
1	G	85	LEU
1	G	125	ASN
1	G	148	ASN
1	G	210	LEU
1	G	255	CYS
1	G	275	VAL
1	G	314	LYS
1	G	355	LEU
1	G	434	LEU
1	G	447	LYS
1	G	497	ILE
1	G	511	ASP
1	G	526	LYS
1	G	542	ASN
1	G	620	TRP
1	G	621	PHE
1	H	60	ILE
1	H	79	GLN
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	497	ILE
1	H	508	LYS
1	H	522	GLU
1	H	523	MET
1	H	559	GLU
1	H	620	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	78	HIS
1	A	79	GLN
1	A	111	ASN
1	A	125	ASN
1	A	129	HIS
1	A	148	ASN
1	A	175	GLN
1	A	211	GLN
1	A	281	HIS
1	A	382	HIS
1	A	423	GLN
1	A	472	GLN
1	A	494	HIS
1	A	577	GLN
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	241	ASN
1	B	423	GLN
1	B	472	GLN
1	B	485	HIS
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	201	HIS
1	C	214	ASN
1	C	423	GLN
1	C	467	HIS
1	C	472	GLN
1	C	494	HIS
1	C	558	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	577	GLN
1	C	583	HIS
1	D	58	GLN
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	214	ASN
1	D	241	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	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	201	HIS
1	E	214	ASN
1	E	423	GLN
1	E	472	GLN
1	E	542	ASN
1	E	558	GLN
1	F	61	HIS
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
1	F	423	GLN
1	F	472	GLN
1	F	558	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	577	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	423	GLN
1	G	472	GLN
1	G	542	ASN
1	G	558	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	423	GLN
1	H	472	GLN
1	H	577	GLN
1	H	583	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (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	A	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	A	702	1	0,6,6	0.00	-	0,9,9	0.00	-
2	CUA	B	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	B	702	1	0,6,6	0.00	-	0,9,9	0.00	-
2	CUA	C	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	C	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	D	639	-	3,5,5	0.58	0	4,5,5	0.49	0
8	N2O	D	640	-	0,2,2	0.00	-	0,1,1	0.00	-
2	CUA	D	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	D	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	E	639	-	3,5,5	0.57	0	4,5,5	0.45	0
7	IMD	E	640	-	3,5,5	0.57	0	4,5,5	0.45	0
2	CUA	E	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	E	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	F	639	-	3,5,5	0.45	0	4,5,5	0.71	0
2	CUA	F	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	F	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	G	639	-	3,5,5	0.48	0	4,5,5	0.49	0
2	CUA	G	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	G	702	1	0,6,6	0.00	-	0,9,9	0.00	-
7	IMD	H	639	-	3,5,5	0.59	0	4,5,5	0.60	0
8	N2O	H	640	-	0,2,2	0.00	-	0,1,1	0.00	-
2	CUA	H	701	1	0,1,1	0.00	-	0,0,0	0.00	-
3	CUK	H	702	1	0,6,6	0.00	-	0,9,9	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CUA	A	701	1	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CUK	A	702	1	-	0/0/8/8	0/1/1/1
2	CUA	B	701	1	-	0/0/0/0	0/0/0/0
3	CUK	B	702	1	-	0/0/8/8	0/1/1/1
2	CUA	C	701	1	-	0/0/0/0	0/0/0/0
3	CUK	C	702	1	-	0/0/8/8	0/1/1/1
7	IMD	D	639	-	-	0/0/0/0	0/1/1/1
8	N2O	D	640	-	-	0/0/0/0	0/0/0/0
2	CUA	D	701	1	-	0/0/0/0	0/0/0/0
3	CUK	D	702	1	-	0/0/8/8	0/1/1/1
7	IMD	E	639	-	-	0/0/0/0	0/1/1/1
7	IMD	E	640	-	-	0/0/0/0	0/1/1/1
2	CUA	E	701	1	-	0/0/0/0	0/0/0/0
3	CUK	E	702	1	-	0/0/8/8	0/1/1/1
7	IMD	F	639	-	-	0/0/0/0	0/1/1/1
2	CUA	F	701	1	-	0/0/0/0	0/0/0/0
3	CUK	F	702	1	-	0/0/8/8	0/1/1/1
7	IMD	G	639	-	-	0/0/0/0	0/1/1/1
2	CUA	G	701	1	-	0/0/0/0	0/0/0/0
3	CUK	G	702	1	-	0/0/8/8	0/1/1/1
7	IMD	H	639	-	-	0/0/0/0	0/1/1/1
8	N2O	H	640	-	-	0/0/0/0	0/0/0/0
2	CUA	H	701	1	-	0/0/0/0	0/0/0/0
3	CUK	H	702	1	-	0/0/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	CUK	1	0
7	D	639	IMD	2	0
8	D	640	N2O	1	0
7	E	639	IMD	1	0
7	E	640	IMD	3	0
7	F	639	IMD	2	0
7	G	639	IMD	2	0
7	H	639	IMD	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	702	CUK	1	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.15	4 (0%) 89 89	18, 30, 52, 61	0
1	B	581/638 (91%)	-0.21	2 (0%) 94 95	15, 27, 46, 57	0
1	C	581/638 (91%)	-0.60	0 100 100	7, 14, 28, 39	0
1	D	588/638 (92%)	-0.50	0 100 100	7, 18, 32, 43	0
1	E	581/638 (91%)	-0.65	0 100 100	7, 11, 23, 31	0
1	F	581/638 (91%)	-0.65	0 100 100	7, 12, 26, 35	0
1	G	585/638 (91%)	-0.45	4 (0%) 89 89	8, 17, 39, 53	0
1	H	581/638 (91%)	-0.56	0 100 100	7, 15, 30, 38	0
All	All	4659/5104 (91%)	-0.47	10 (0%) 95 96	7, 18, 40, 61	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	551	MET	3.2
1	G	264	LEU	2.6
1	A	638	ALA	2.6
1	G	494	HIS	2.4
1	G	309	ASP	2.4
1	A	207	VAL	2.3
1	A	578	ILE	2.2
1	B	624	ALA	2.2
1	G	238	ASN	2.1
1	A	580	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	IMD	D	639	5/5	0.96	0.24	7.59	27,27,28,28	0
8	N2O	D	640	3/3	0.97	0.36	7.02	43,43,44,45	0
7	IMD	F	639	5/5	0.94	0.22	5.41	32,33,33,34	0
8	N2O	H	640	3/3	0.93	0.40	4.62	51,51,51,52	0
7	IMD	E	640	5/5	0.98	0.13	3.88	12,12,14,14	0
7	IMD	H	639	5/5	0.97	0.13	1.96	11,13,14,14	0
7	IMD	G	639	5/5	0.92	0.24	1.70	27,28,28,28	0
5	CL	B	704	1/1	0.97	0.19	0.63	45,45,45,45	0
5	CL	A	704	1/1	0.95	0.18	0.58	39,39,39,39	0
6	K	G	705	1/1	0.43	0.18	0.48	57,57,57,57	0
3	CUK	H	702	6/6	0.91	0.13	0.24	32,36,39,41	6
3	CUK	B	702	6/6	0.83	0.15	-0.08	51,53,55,57	6
4	CA	H	703	1/1	0.96	0.09	-0.39	9,9,9,9	0
4	CA	E	703	1/1	0.99	0.08	-0.47	10,10,10,10	0
3	CUK	C	702	6/6	0.97	0.11	-0.57	27,31,34,34	6
6	K	E	705	1/1	0.71	0.10	-0.81	55,55,55,55	0
5	CL	D	704	1/1	1.00	0.10	-0.83	25,25,25,25	0
6	K	B	705	1/1	0.91	0.15	-0.84	62,62,62,62	0
5	CL	H	704	1/1	0.99	0.08	-0.86	27,27,27,27	0
5	CL	C	704	1/1	0.99	0.07	-0.89	24,24,24,24	0
3	CUK	E	702	6/6	0.96	0.08	-1.08	27,32,35,36	6
3	CUK	G	702	6/6	0.95	0.10	-1.13	33,38,40,42	6
4	CA	F	703	1/1	0.99	0.04	-1.36	13,13,13,13	0
6	K	H	705	1/1	0.77	0.10	-1.42	56,56,56,56	0
6	K	F	705	1/1	0.90	0.07	-1.45	30,30,30,30	0
6	K	D	705	1/1	0.83	0.09	-1.48	42,42,42,42	0
4	CA	D	703	1/1	0.99	0.05	-1.48	19,19,19,19	0
3	CUK	A	702	6/6	0.95	0.10	-1.56	42,45,47,47	6
6	K	A	705	1/1	0.79	0.11	-1.59	56,56,56,56	0
6	K	C	705	1/1	0.85	0.09	-1.66	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CUA	G	701	2/2	0.99	0.07	-1.66	15,15,15,18	0
4	CA	C	703	1/1	0.99	0.05	-1.70	11,11,11,11	0
5	CL	E	704	1/1	0.99	0.05	-1.70	20,20,20,20	0
2	CUA	D	701	2/2	0.98	0.07	-1.70	17,17,17,18	0
5	CL	G	704	1/1	1.00	0.05	-1.74	26,26,26,26	0
2	CUA	H	701	2/2	0.97	0.06	-1.75	29,29,29,31	0
2	CUA	F	701	2/2	0.98	0.07	-1.82	18,18,18,21	0
4	CA	A	703	1/1	0.93	0.08	-1.85	37,37,37,37	0
4	CA	B	703	1/1	0.99	0.06	-1.87	23,23,23,23	0
2	CUA	E	701	2/2	0.99	0.06	-1.88	14,14,14,17	0
3	CUK	F	702	6/6	0.97	0.07	-1.88	22,27,28,29	5
3	CUK	D	702	6/6	0.96	0.06	-2.10	27,32,32,35	6
2	CUA	A	701	2/2	0.96	0.06	-2.10	30,30,30,33	0
2	CUA	C	701	2/2	0.96	0.07	-2.20	21,21,21,25	0
5	CL	F	704	1/1	0.99	0.04	-2.37	17,17,17,17	0
4	CA	G	703	1/1	0.97	0.05	-3.07	31,31,31,31	0
2	CUA	B	701	2/2	0.98	0.04	-3.49	37,37,37,38	0
7	IMD	E	639	5/5	0.97	0.10	-	26,27,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.