



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:47 pm BST

PDB ID : 1QNI
Title : Crystal Structure of Nitrous Oxide Reductase from *Pseudomonas nautica*, at 2.4Å Resolution
Authors : Brown, K.; Tegoni, M.; Cambillau, C.
Deposited on : 1999-10-15
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

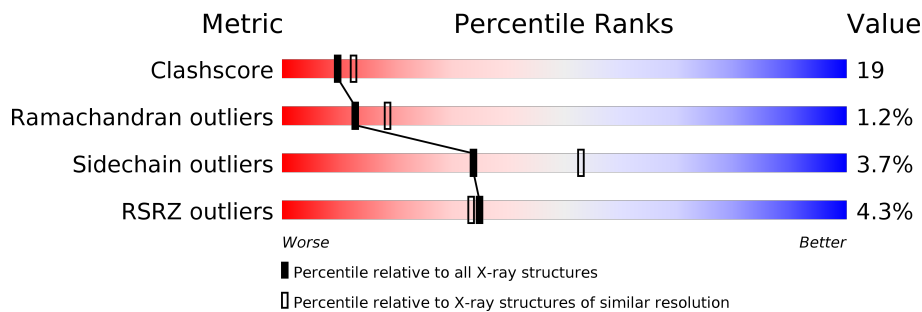
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	581	 3% 68% 28% ..
1	B	581	 4% 68% 27% ..
1	C	581	 7% 61% 35% ..
1	D	581	 3% 62% 34% ..
1	E	581	 4% 66% 31% ..
1	F	581	 4% 64% 31% ..

2 Entry composition [i](#)

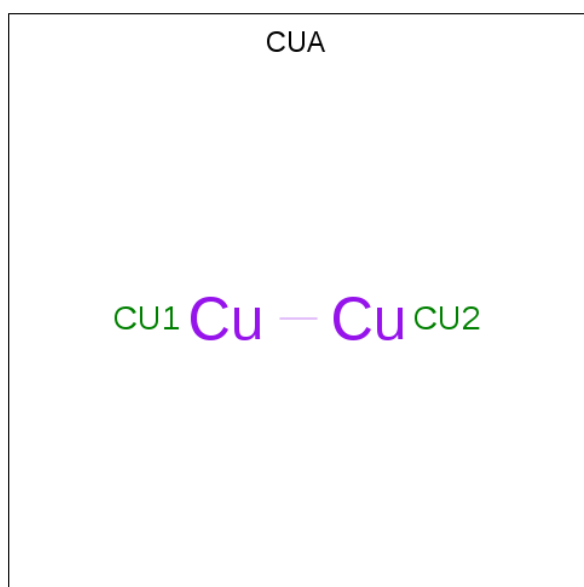
There are 6 unique types of molecules in this entry. The entry contains 28448 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

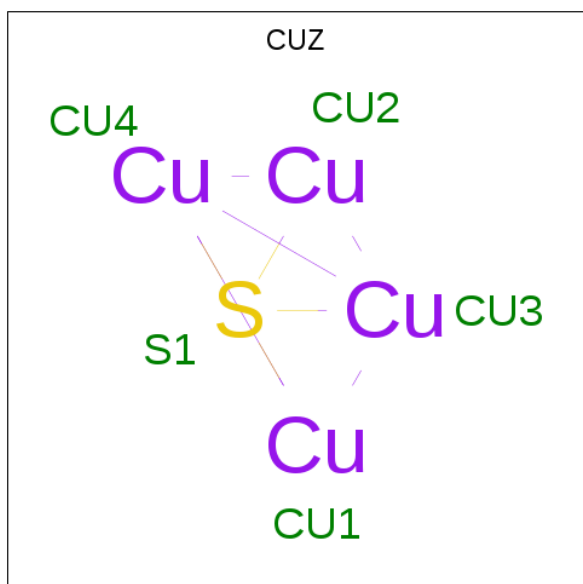
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	572	Total 4513	C 2842	N 779	O 867	S 25	8	0	0
1	B	572	Total 4513	C 2842	N 779	O 867	S 25	8	0	0
1	C	572	Total 4513	C 2842	N 779	O 867	S 25	8	0	0
1	D	572	Total 4513	C 2842	N 779	O 867	S 25	8	0	0
1	E	572	Total 4513	C 2842	N 779	O 867	S 25	8	0	0
1	F	572	Total 4513	C 2842	N 779	O 867	S 25	8	0	0

- Molecule 2 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 3 is (MU-4-SULFIDO)-TETRA-NUCLEAR COPPER ION (three-letter code: CUZ) (formula: Cu₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cu S 5 4 1	0	0
3	B	1	Total Cu S 5 4 1	0	0
3	C	1	Total Cu S 5 4 1	0	0
3	D	1	Total Cu S 5 4 1	0	0
3	E	1	Total Cu S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	F	1	Total	Cu	S	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Ca	0	0
			2	2		
4	E	2	Total	Ca	0	0
			2	2		
4	B	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	A	2	Total	Ca	0	0
			2	2		
4	F	2	Total	Ca	0	0
			2	2		

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	332	Total	O	0	0
			332	332		
6	B	317	Total	O	0	0
			317	317		

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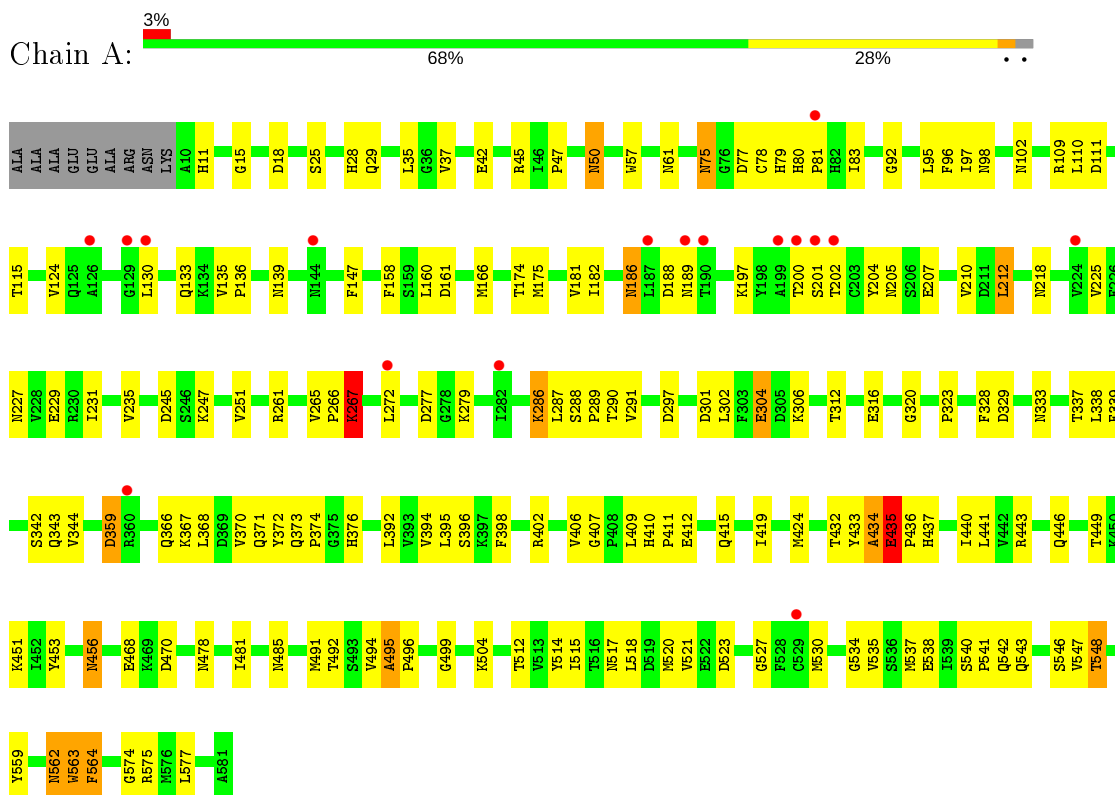
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	97	Total 97	O 97	0	0
6	D	116	Total 116	O 116	0	0
6	E	223	Total 223	O 223	0	0
6	F	225	Total 225	O 225	0	0

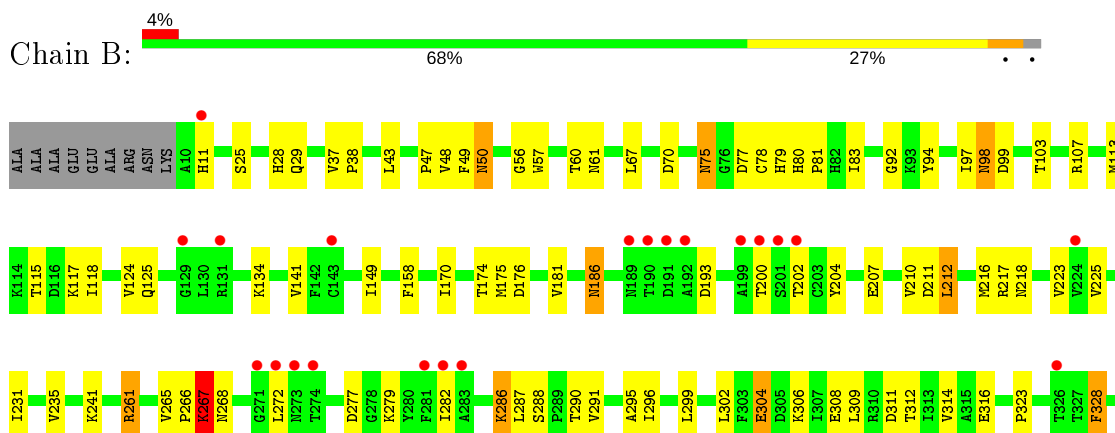
3 Residue-property plots

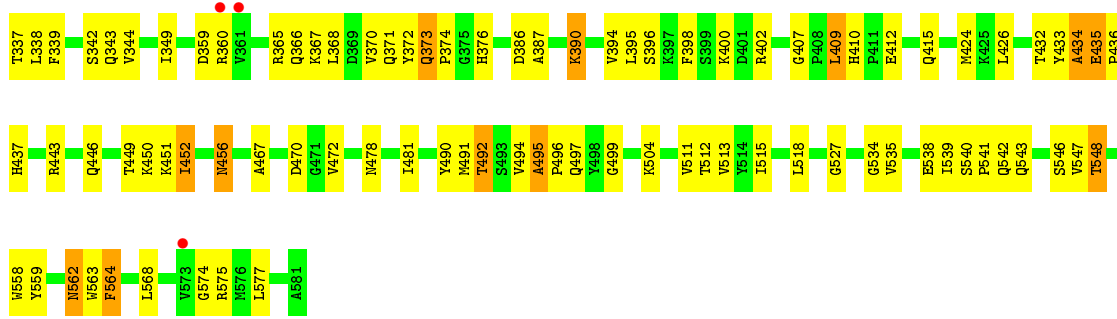
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NITROUS-OXIDE REDUCTASE

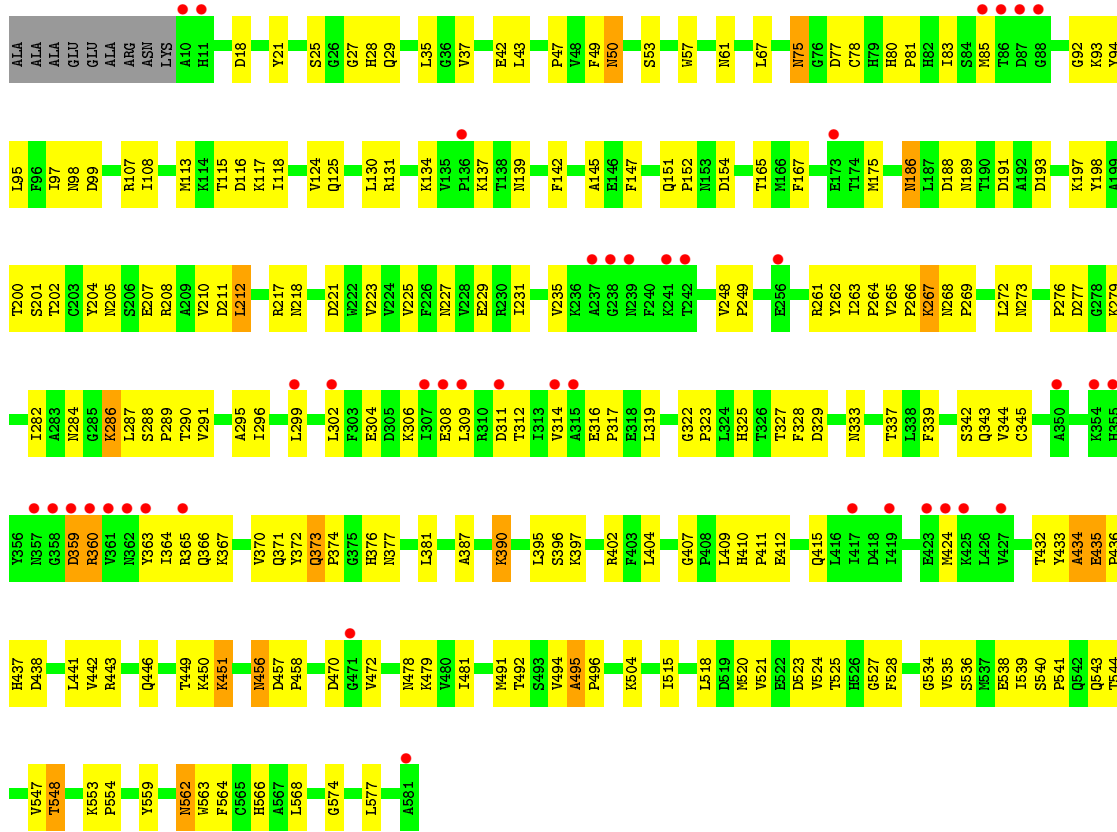


• Molecule 1: NITROUS-OXIDE REDUCTASE

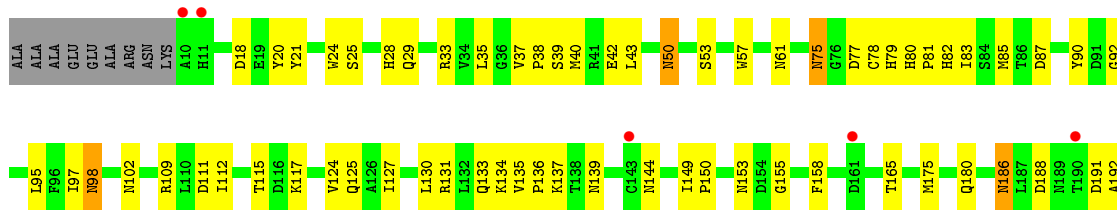


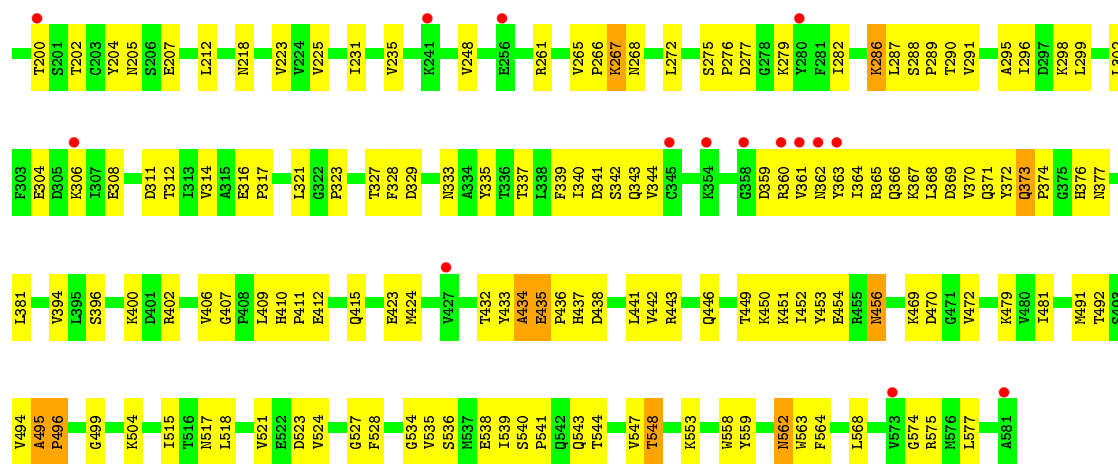


• Molecule 1: NITROUS-OXIDE REDUCTASE

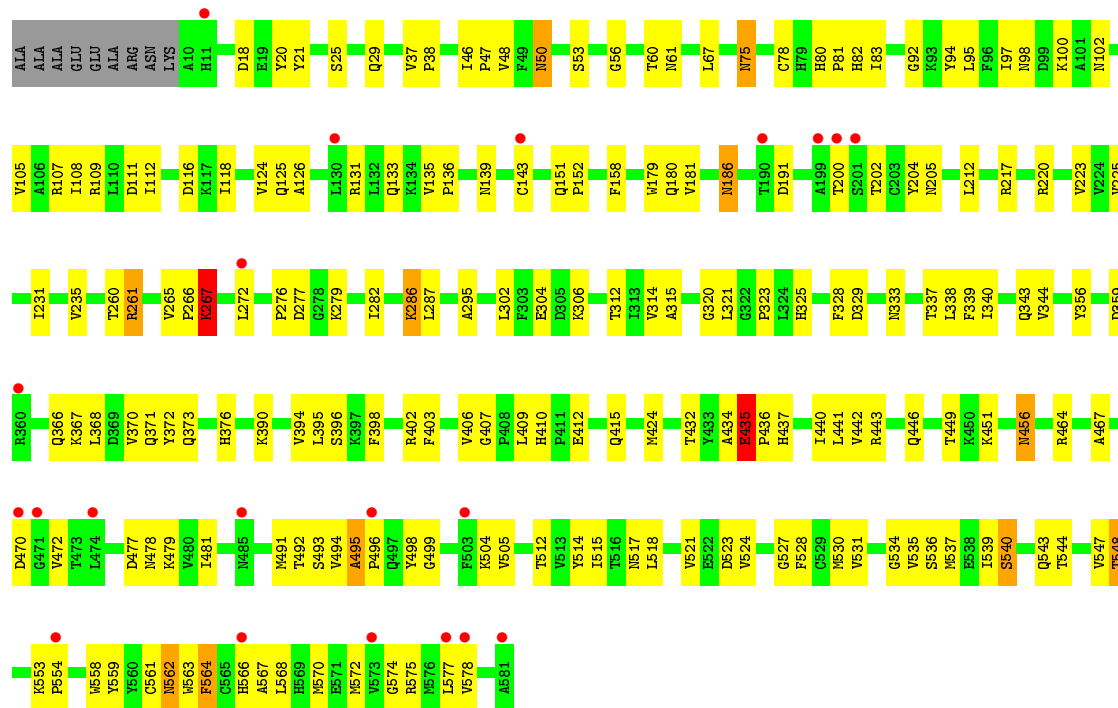


• Molecule 1: NITROUS-OXIDE REDUCTASE

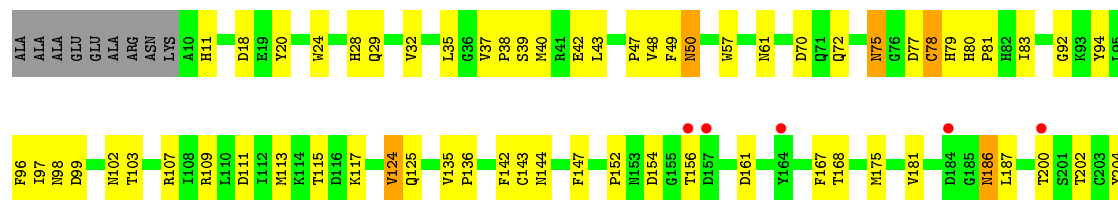


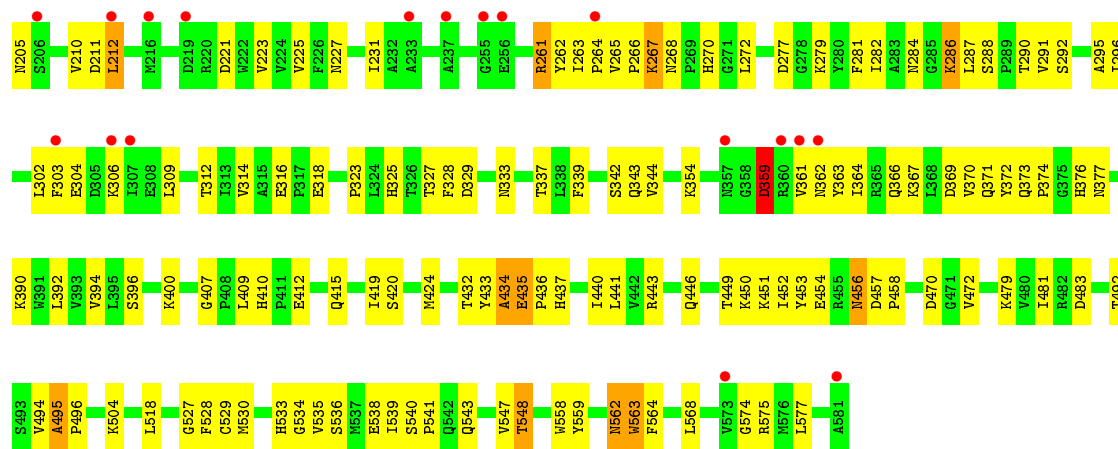


• Molecule 1: NITROUS-OXIDE REDUCTASE



• Molecule 1: NITROUS-OXIDE REDUCTASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	211.29Å 211.29Å 166.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.7 (20.00-2.40) 90.8 (30.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.39Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.228 , 0.261 0.223 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtrriage
Anisotropy	0.564	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28448	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/4619	0.67	2/6271 (0.0%)
1	B	0.38	0/4619	0.68	1/6271 (0.0%)
1	C	0.35	0/4619	0.61	0/6271
1	D	0.36	0/4619	0.62	0/6271
1	E	0.38	0/4619	0.67	2/6271 (0.0%)
1	F	0.38	0/4619	0.65	0/6271
All	All	0.37	0/27714	0.65	5/37626 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	LYS	N-CA-C	5.93	127.02	111.00
1	E	267	LYS	N-CA-C	5.86	126.82	111.00
1	E	435	GLU	N-CA-C	5.43	125.66	111.00
1	A	267	LYS	N-CA-C	5.37	125.50	111.00
1	A	435	GLU	N-CA-C	5.35	125.43	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4513	0	4356	162	0
1	B	4513	0	4356	180	0
1	C	4513	0	4356	187	0
1	D	4513	0	4356	191	0
1	E	4513	0	4356	169	0
1	F	4513	0	4356	191	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
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	332	0	0	16	0
6	B	317	0	0	16	0
6	C	97	0	0	4	0
6	D	116	0	0	6	0
6	E	223	0	0	14	0
6	F	225	0	0	24	0
All	All	28448	0	26136	1018	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 19.

All (1018) 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:F:83:ILE:HD11	1:F:92:GLY:HA2	1.37	1.01
1:C:83:ILE:HD11	1:C:92:GLY:HA2	1.44	0.99
1:E:443:ARG:H	1:E:446:GLN:HE21	1.09	0.98
1:E:564:PHE:HE2	6:F:2094:HOH:O	1.49	0.95
1:B:366:GLN:HE22	1:B:424:MET:H	1.02	0.95
1:A:371:GLN:H	1:A:415:GLN:HE22	1.15	0.94
1:C:371:GLN:H	1:C:415:GLN:HE22	1.12	0.94
1:D:371:GLN:H	1:D:415:GLN:HE22	0.94	0.93
1:E:371:GLN:H	1:E:415:GLN:HE22	1.13	0.93
1:B:443:ARG:H	1:B:446:GLN:HE21	1.05	0.92
1:E:564:PHE:CE2	6:F:2094:HOH:O	2.21	0.92
1:D:83:ILE:HD11	1:D:92:GLY:HA2	1.50	0.91
1:D:443:ARG:H	1:D:446:GLN:HE21	0.94	0.90
1:A:75:ASN:HD21	1:B:534:GLY:HA2	1.34	0.89
1:F:443:ARG:H	1:F:446:GLN:HE21	1.16	0.88
1:A:534:GLY:HA2	1:B:75:ASN:HD21	1.36	0.88
1:C:443:ARG:H	1:C:446:GLN:HE21	1.17	0.88
1:D:366:GLN:HE22	1:D:424:MET:H	1.18	0.88
1:E:50:ASN:HD22	1:E:50:ASN:H	1.13	0.88
1:E:200:THR:HG22	1:E:225:VAL:HA	1.57	0.87
1:F:568:LEU:HA	6:F:2218:HOH:O	1.73	0.87
1:A:83:ILE:HD11	1:A:92:GLY:HA2	1.56	0.87
1:F:371:GLN:H	1:F:415:GLN:HE22	1.18	0.87
1:E:366:GLN:HE22	1:E:424:MET:H	1.20	0.86
1:C:535:VAL:HG13	1:C:547:VAL:HG21	1.55	0.86
1:E:75:ASN:HD21	1:F:534:GLY:HA2	1.38	0.86
1:D:371:GLN:H	1:D:415:GLN:NE2	1.74	0.85
1:B:371:GLN:H	1:B:415:GLN:HE22	1.21	0.85
1:E:495:ALA:HB1	1:E:496:PRO:HD2	1.56	0.85
1:A:366:GLN:HE22	1:A:424:MET:H	1.23	0.84
1:B:50:ASN:H	1:B:50:ASN:HD22	1.21	0.84
1:F:50:ASN:H	1:F:50:ASN:HD22	1.25	0.84
1:C:366:GLN:HE22	1:C:424:MET:H	1.24	0.84
1:C:412:GLU:HG3	1:C:435:GLU:HA	1.60	0.83
1:C:495:ALA:HB1	1:C:496:PRO:HD2	1.58	0.83
1:A:50:ASN:HD22	1:A:50:ASN:H	1.23	0.83
1:D:443:ARG:N	1:D:446:GLN:HE21	1.77	0.82
1:A:344:VAL:HG23	1:A:370:VAL:HG21	1.58	0.82
1:B:61:ASN:HD21	1:B:548:THR:HG23	1.41	0.82
1:A:443:ARG:H	1:A:446:GLN:HE21	1.28	0.82
1:C:75:ASN:HD21	1:D:534:GLY:HA2	1.45	0.81
1:D:304:GLU:HG2	1:D:306:LYS:HE2	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:344:VAL:HG23	1:F:370:VAL:HG21	1.60	0.81
1:D:443:ARG:H	1:D:446:GLN:NE2	1.75	0.80
1:D:495:ALA:HB1	1:D:496:PRO:CD	2.11	0.80
1:B:277:ASP:OD1	1:B:279:LYS:HG2	1.82	0.80
1:B:470:ASP:HB3	1:B:481:ILE:HD13	1.62	0.79
1:A:495:ALA:HB1	1:A:496:PRO:CD	2.12	0.79
1:F:61:ASN:HD21	1:F:548:THR:HG22	1.46	0.78
1:E:83:ILE:HD11	1:E:92:GLY:HA2	1.65	0.78
1:D:432:THR:HG21	1:D:436:PRO:HG3	1.64	0.78
1:F:495:ALA:HB1	1:F:496:PRO:CD	2.14	0.78
1:E:535:VAL:HG13	1:E:547:VAL:HG21	1.66	0.77
1:B:495:ALA:HB1	1:B:496:PRO:CD	2.14	0.77
1:D:200:THR:HG22	1:D:225:VAL:HA	1.67	0.77
1:E:75:ASN:ND2	1:F:534:GLY:HA2	1.97	0.77
1:B:83:ILE:HD11	1:B:92:GLY:HA2	1.66	0.77
1:D:535:VAL:HG13	1:D:547:VAL:HG21	1.66	0.77
1:F:80:HIS:H	1:F:98:ASN:ND2	1.82	0.76
1:D:495:ALA:HB1	1:D:496:PRO:HD2	1.66	0.76
1:A:200:THR:HG22	1:A:225:VAL:HA	1.67	0.76
1:C:50:ASN:H	1:C:50:ASN:HD22	1.33	0.76
1:D:527:GLY:HA3	1:D:562:ASN:ND2	2.01	0.75
1:F:568:LEU:HD23	6:F:2218:HOH:O	1.86	0.75
1:F:61:ASN:HD21	1:F:548:THR:CG2	1.99	0.75
1:B:443:ARG:H	1:B:446:GLN:NE2	1.84	0.74
1:C:495:ALA:HB1	1:C:496:PRO:CD	2.17	0.74
1:F:343:GLN:NE2	1:F:367:LYS:HD3	2.03	0.74
1:B:79:HIS:H	1:B:98:ASN:HD21	1.34	0.74
6:A:2297:HOH:O	1:B:211:ASP:HB3	1.87	0.73
1:C:302:LEU:HD11	1:C:309:LEU:HD23	1.70	0.73
1:A:470:ASP:HB3	1:A:481:ILE:HD13	1.71	0.73
1:E:540:SER:H	1:E:543:GLN:HE21	1.37	0.73
1:B:304:GLU:HG2	1:B:306:LYS:HE2	1.71	0.73
1:E:50:ASN:ND2	1:E:50:ASN:H	1.86	0.73
1:C:200:THR:HG22	1:C:225:VAL:HA	1.70	0.72
1:C:277:ASP:OD1	1:C:279:LYS:HG2	1.88	0.72
1:B:11:HIS:HA	6:B:2001:HOH:O	1.90	0.72
1:B:67:LEU:HD23	1:B:118:ILE:HD13	1.71	0.72
1:B:366:GLN:HE22	1:B:424:MET:N	1.84	0.72
1:B:443:ARG:HB2	1:B:446:GLN:HG3	1.70	0.72
1:D:527:GLY:HA3	1:D:562:ASN:HD21	1.54	0.72
1:B:267:LYS:HB3	1:B:287:LEU:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:VAL:HG23	1:C:370:VAL:HG21	1.72	0.72
1:A:495:ALA:HB1	1:A:496:PRO:HD2	1.72	0.72
1:A:75:ASN:ND2	1:B:534:GLY:HA2	2.05	0.72
1:D:75:ASN:HD21	1:D:102:ASN:HD21	1.38	0.71
1:B:443:ARG:N	1:B:446:GLN:HE21	1.85	0.71
1:F:443:ARG:N	1:F:446:GLN:HE21	1.88	0.71
1:B:412:GLU:HG3	1:B:435:GLU:HA	1.72	0.71
1:A:540:SER:H	1:A:543:GLN:NE2	1.89	0.70
1:D:75:ASN:ND2	1:D:102:ASN:HD21	1.88	0.70
1:D:412:GLU:HG3	1:D:435:GLU:HA	1.73	0.70
1:E:344:VAL:HG23	1:E:370:VAL:HG21	1.71	0.70
1:E:329:ASP:OD2	1:E:333:ASN:HB2	1.92	0.70
1:A:61:ASN:OD1	1:A:548:THR:HG22	1.92	0.69
1:C:443:ARG:HB2	1:C:446:GLN:HG3	1.74	0.69
1:D:371:GLN:HG2	1:D:402:ARG:HD2	1.74	0.69
1:E:29:GLN:HB2	1:E:434:ALA:CB	2.23	0.69
1:C:504:LYS:HG2	1:C:577:LEU:HB2	1.74	0.69
1:E:223:VAL:HG23	1:E:265:VAL:HG21	1.75	0.69
1:E:456:ASN:H	1:E:456:ASN:HD22	1.39	0.69
1:C:186:ASN:HD21	1:C:204:TYR:H	1.39	0.69
1:B:366:GLN:NE2	1:B:424:MET:H	1.83	0.69
1:F:38:PRO:HB2	6:F:2002:HOH:O	1.93	0.69
1:F:366:GLN:HE22	1:F:424:MET:H	1.38	0.69
1:B:344:VAL:HG23	1:B:370:VAL:HG21	1.74	0.69
1:D:344:VAL:HG23	1:D:370:VAL:HG21	1.74	0.68
1:F:443:ARG:HB2	1:F:446:GLN:HG3	1.75	0.68
1:B:495:ALA:HB1	1:B:496:PRO:HD2	1.74	0.68
1:E:410:HIS:CE1	1:F:451:LYS:HE3	2.28	0.68
1:D:79:HIS:H	1:D:98:ASN:HD21	1.40	0.68
1:A:534:GLY:HA2	1:B:75:ASN:ND2	2.07	0.68
1:A:80:HIS:H	1:A:98:ASN:ND2	1.92	0.68
1:B:29:GLN:HB2	1:B:434:ALA:CB	2.24	0.68
1:F:304:GLU:HG2	1:F:306:LYS:HE2	1.74	0.68
1:A:366:GLN:NE2	1:A:424:MET:H	1.92	0.68
1:E:443:ARG:HB2	1:E:446:GLN:HG3	1.75	0.68
1:C:371:GLN:HG2	1:C:402:ARG:HD2	1.74	0.68
1:C:559:TYR:CZ	1:C:574:GLY:HA3	2.29	0.68
6:A:2290:HOH:O	1:E:477:ASP:HA	1.94	0.68
1:F:83:ILE:HD11	1:F:92:GLY:CA	2.19	0.68
1:E:75:ASN:ND2	1:E:102:ASN:HD21	1.92	0.67
1:F:412:GLU:HG3	1:F:435:GLU:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:483:ASP:HA	6:F:2177:HOH:O	1.93	0.67
1:D:540:SER:H	1:D:543:GLN:HE21	1.43	0.67
1:E:267:LYS:HB3	1:E:287:LEU:HB2	1.76	0.67
1:E:261:ARG:HG2	1:E:302:LEU:HG	1.75	0.67
1:F:267:LYS:HB3	1:F:287:LEU:HB2	1.75	0.67
1:A:443:ARG:HB2	1:A:446:GLN:HG3	1.76	0.67
1:F:450:LYS:HD3	6:F:2151:HOH:O	1.95	0.67
1:C:527:GLY:HA3	1:C:562:ASN:ND2	2.10	0.67
1:F:443:ARG:H	1:F:446:GLN:NE2	1.92	0.67
1:D:504:LYS:HG2	1:D:577:LEU:HB2	1.76	0.67
1:B:80:HIS:H	1:B:98:ASN:ND2	1.93	0.67
1:C:496:PRO:HD3	1:C:566:HIS:CD2	2.30	0.67
1:E:75:ASN:HD21	1:E:102:ASN:HD21	1.43	0.66
1:A:478:ASN:HD21	1:A:492:THR:HG22	1.59	0.66
1:F:472:VAL:HG12	1:F:479:LYS:HD2	1.77	0.66
1:A:78:CYS:HB2	1:A:97:ILE:CD1	2.25	0.66
1:B:504:LYS:HG2	1:B:577:LEU:HB2	1.76	0.66
1:F:286:LYS:H	1:F:323:PRO:HG2	1.60	0.66
1:D:366:GLN:NE2	1:D:424:MET:H	1.92	0.66
1:D:329:ASP:OD2	1:D:333:ASN:HB2	1.95	0.65
1:E:534:GLY:HA2	1:F:75:ASN:HD21	1.61	0.65
1:D:277:ASP:OD1	1:D:279:LYS:HG2	1.96	0.65
1:E:540:SER:H	1:E:543:GLN:NE2	1.92	0.65
1:C:267:LYS:HB3	1:C:287:LEU:HB2	1.78	0.65
1:B:268:ASN:O	1:B:286:LYS:HE2	1.97	0.65
1:E:304:GLU:HG2	1:E:306:LYS:HE2	1.78	0.65
1:F:540:SER:H	1:F:543:GLN:NE2	1.95	0.65
1:F:453:TYR:CD2	1:F:543:GLN:HB2	2.32	0.64
1:B:48:VAL:H	1:B:50:ASN:ND2	1.95	0.64
1:B:61:ASN:ND2	1:B:548:THR:HG23	2.11	0.64
1:E:495:ALA:HB1	1:E:496:PRO:CD	2.28	0.64
1:F:270:HIS:CE1	3:F:801:CUZ:S1	2.91	0.64
1:A:491:MET:HB2	1:A:515:ILE:HD13	1.79	0.64
1:C:456:ASN:HD22	1:C:456:ASN:H	1.45	0.64
1:C:527:GLY:HA3	1:C:562:ASN:HD21	1.63	0.64
1:D:562:ASN:H	1:D:562:ASN:ND2	1.96	0.64
1:F:186:ASN:HD21	1:F:204:TYR:H	1.46	0.64
1:A:449:THR:HG21	1:B:407:GLY:N	2.13	0.64
1:C:540:SER:H	1:C:543:GLN:NE2	1.97	0.63
1:D:286:LYS:H	1:D:323:PRO:HG2	1.61	0.63
1:F:20:TYR:HB2	1:F:37:VAL:HB	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:ASP:OD2	1:C:333:ASN:HB2	1.98	0.63
1:A:344:VAL:HG21	1:A:394:VAL:HG21	1.79	0.63
1:C:61:ASN:HD21	1:C:548:THR:CG2	2.11	0.63
1:D:443:ARG:HB2	1:D:446:GLN:HG3	1.79	0.63
1:A:406:VAL:O	1:B:113:MET:HG3	1.99	0.63
1:B:50:ASN:ND2	1:B:50:ASN:H	1.92	0.63
1:E:344:VAL:HG21	1:E:394:VAL:HG21	1.81	0.63
1:F:61:ASN:ND2	1:F:548:THR:HG22	2.13	0.63
1:A:50:ASN:ND2	1:A:50:ASN:H	1.95	0.63
1:E:443:ARG:H	1:E:446:GLN:NE2	1.90	0.63
1:F:344:VAL:HG23	1:F:370:VAL:CG2	2.29	0.63
1:D:50:ASN:HD22	1:D:50:ASN:H	1.46	0.63
1:C:223:VAL:HG23	1:C:265:VAL:HG21	1.81	0.62
1:D:559:TYR:CZ	1:D:574:GLY:HA3	2.34	0.62
1:E:277:ASP:OD1	1:E:279:LYS:HG2	1.99	0.62
1:A:432:THR:HG21	1:A:436:PRO:HG3	1.80	0.62
1:D:366:GLN:HE22	1:D:424:MET:N	1.94	0.62
1:E:25:SER:HB3	1:E:81:PRO:HD3	1.81	0.62
1:E:559:TYR:CZ	1:E:574:GLY:HA3	2.34	0.62
1:D:371:GLN:N	1:D:415:GLN:HE22	1.80	0.62
1:F:94:TYR:CD1	1:F:107:ARG:HD3	2.35	0.62
1:A:517:ASN:HD22	1:A:540:SER:C	2.03	0.62
1:C:145:ALA:HB3	1:C:165:THR:OG1	2.00	0.62
1:E:527:GLY:HA3	1:E:562:ASN:ND2	2.15	0.62
1:A:320:GLY:HA3	1:A:338:LEU:HD13	1.82	0.61
1:B:181:VAL:HG21	1:B:231:ILE:HD13	1.82	0.61
1:C:407:GLY:H	1:D:449:THR:HG21	1.65	0.61
1:D:540:SER:H	1:D:543:GLN:NE2	1.97	0.61
1:E:504:LYS:HG2	1:E:577:LEU:HB2	1.80	0.61
1:A:412:GLU:HG3	1:A:435:GLU:HA	1.82	0.61
1:D:20:TYR:HB2	1:D:37:VAL:HB	1.81	0.61
1:B:456:ASN:HD22	1:B:456:ASN:H	1.48	0.61
1:E:50:ASN:N	1:E:50:ASN:HD22	1.94	0.61
1:C:304:GLU:HB3	1:C:306:LYS:HG3	1.82	0.61
1:E:29:GLN:HB2	1:E:434:ALA:HB1	1.81	0.61
1:F:28:HIS:HA	1:F:77:ASP:HA	1.83	0.61
1:A:186:ASN:HD21	1:A:204:TYR:H	1.48	0.61
1:C:443:ARG:H	1:C:446:GLN:NE2	1.94	0.61
1:C:451:LYS:HE2	1:D:410:HIS:NE2	2.15	0.61
1:A:495:ALA:CB	1:A:496:PRO:CD	2.79	0.61
1:E:470:ASP:HB3	1:E:481:ILE:CD1	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ASN:O	1:D:286:LYS:HE2	2.00	0.61
1:D:495:ALA:CB	1:D:496:PRO:CD	2.78	0.61
1:F:495:ALA:CB	1:F:496:PRO:CD	2.78	0.61
1:E:186:ASN:HD21	1:E:204:TYR:H	1.49	0.60
1:E:493:SER:O	1:E:494:VAL:HG13	2.01	0.60
1:E:492:THR:HG22	1:E:499:GLY:HA3	1.81	0.60
1:E:496:PRO:HD3	1:E:566:HIS:CD2	2.36	0.60
1:A:395:LEU:N	1:A:395:LEU:HD12	2.15	0.60
1:D:344:VAL:HG23	1:D:370:VAL:CG2	2.31	0.60
1:A:407:GLY:H	1:B:449:THR:HG21	1.66	0.60
1:A:79:HIS:H	1:A:98:ASN:HD21	1.49	0.60
1:C:202:THR:HG23	1:C:272:LEU:HB2	1.82	0.60
1:C:295:ALA:HB2	1:C:314:VAL:CG2	2.32	0.60
1:F:327:THR:HG22	1:F:377:ASN:ND2	2.16	0.60
1:F:372:TYR:O	1:F:396:SER:HB3	2.01	0.60
1:E:410:HIS:HE1	1:F:451:LYS:HE3	1.67	0.59
1:F:495:ALA:HB1	1:F:496:PRO:HD2	1.84	0.59
1:C:227:ASN:O	1:C:231:ILE:HG13	2.02	0.59
1:C:67:LEU:HD23	1:C:118:ILE:CD1	2.32	0.59
1:B:200:THR:HG22	1:B:225:VAL:HG22	1.85	0.59
1:C:295:ALA:HB2	1:C:314:VAL:HG21	1.84	0.59
1:D:61:ASN:HD21	1:D:548:THR:CG2	2.14	0.59
1:E:412:GLU:HG3	1:E:435:GLU:HA	1.84	0.59
1:B:323:PRO:HA	1:B:337:THR:O	2.02	0.59
1:F:181:VAL:HG21	1:F:231:ILE:HD13	1.84	0.59
1:A:200:THR:CG2	1:A:225:VAL:HG22	2.33	0.59
1:E:343:GLN:NE2	1:E:367:LYS:HD3	2.17	0.59
1:F:202:THR:HG23	1:F:272:LEU:HB2	1.84	0.59
1:B:527:GLY:HA3	1:B:562:ASN:ND2	2.17	0.59
1:C:470:ASP:HB3	1:C:481:ILE:HD13	1.84	0.59
1:B:202:THR:HG23	1:B:272:LEU:HB2	1.84	0.59
1:D:265:VAL:HG13	1:D:266:PRO:HD2	1.83	0.59
1:B:376:HIS:HB2	1:B:437:HIS:O	2.03	0.59
1:E:491:MET:HB2	1:E:515:ILE:HD13	1.85	0.59
1:B:512:THR:HG23	1:B:548:THR:HG22	1.84	0.59
1:F:291:VAL:O	1:F:316:GLU:HA	2.03	0.59
1:F:47:PRO:HA	1:F:50:ASN:HD21	1.67	0.59
1:A:109:ARG:HD2	1:A:111:ASP:OD1	2.03	0.58
1:C:61:ASN:HD21	1:C:548:THR:HG22	1.68	0.58
1:E:48:VAL:H	1:E:50:ASN:ND2	2.02	0.58
1:A:540:SER:H	1:A:543:GLN:HE21	1.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:THR:HB	1:D:374:PRO:HB2	1.83	0.58
1:A:468:GLU:HB2	6:A:2275:HOH:O	2.03	0.58
1:C:344:VAL:HG23	1:C:370:VAL:CG2	2.34	0.58
1:C:371:GLN:H	1:C:415:GLN:NE2	1.93	0.58
1:E:373:GLN:HE21	1:E:398:PHE:HD2	1.48	0.58
1:E:83:ILE:HB	6:E:2028:HOH:O	2.03	0.58
1:A:366:GLN:HE22	1:A:424:MET:N	1.99	0.58
1:B:79:HIS:H	1:B:98:ASN:ND2	2.01	0.58
1:C:538:GLU:C	1:C:539:ILE:HG13	2.23	0.58
1:E:478:ASN:HD21	1:E:492:THR:CG2	2.17	0.58
1:A:207:GLU:HG3	1:A:218:ASN:ND2	2.19	0.58
1:F:290:THR:HG22	1:F:318:GLU:HA	1.86	0.58
1:C:521:VAL:HB	1:C:524:VAL:HG21	1.84	0.58
1:C:534:GLY:HA2	1:D:75:ASN:HD21	1.68	0.58
1:C:342:SER:HA	1:C:374:PRO:HD3	1.84	0.58
1:C:75:ASN:HD22	1:C:75:ASN:H	1.51	0.58
1:C:525:THR:HG23	1:C:540:SER:HA	1.85	0.58
1:E:570:MET:HG3	6:F:2098:HOH:O	2.03	0.58
1:C:540:SER:H	1:C:543:GLN:HE21	1.51	0.57
1:F:494:VAL:HG12	1:F:518:LEU:HB2	1.86	0.57
1:C:472:VAL:HG12	1:C:479:LYS:HD2	1.86	0.57
1:E:323:PRO:HA	1:E:337:THR:O	2.03	0.57
1:A:25:SER:HB3	1:A:81:PRO:HD3	1.85	0.57
1:F:35:LEU:HD22	1:F:42:GLU:HA	1.85	0.57
1:A:371:GLN:HG2	1:A:402:ARG:NH1	2.19	0.57
1:C:395:LEU:HD22	1:C:437:HIS:O	2.04	0.57
1:F:302:LEU:HD22	1:F:312:THR:HG21	1.85	0.57
1:A:231:ILE:O	1:A:235:VAL:HG23	2.04	0.57
1:C:261:ARG:HG2	1:C:302:LEU:HG	1.85	0.57
1:F:282:ILE:HG23	1:F:291:VAL:HG13	1.86	0.57
1:D:562:ASN:H	1:D:562:ASN:HD22	1.52	0.57
1:E:498:TYR:CE1	1:E:572:MET:HG2	2.39	0.57
1:A:504:LYS:HG2	1:A:577:LEU:HB2	1.86	0.57
1:C:540:SER:HB3	1:C:541:PRO:HD2	1.85	0.57
1:D:186:ASN:H	1:D:186:ASN:HD22	1.51	0.57
1:A:453:TYR:CD2	1:A:543:GLN:HB2	2.39	0.57
1:D:25:SER:HB3	1:D:81:PRO:HD3	1.87	0.57
1:F:279:LYS:HB2	6:F:2096:HOH:O	2.03	0.57
1:C:410:HIS:HB2	1:D:523:ASP:OD1	2.05	0.57
1:C:80:HIS:H	1:C:98:ASN:ND2	2.03	0.57
1:E:339:PHE:CE1	1:E:373:GLN:HB3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:CG2	1:B:225:VAL:HG22	2.34	0.56
1:C:491:MET:HB2	1:C:515:ILE:HD13	1.88	0.56
1:E:478:ASN:HD21	1:E:492:THR:HG22	1.70	0.56
1:F:81:PRO:HB3	1:F:97:ILE:HD12	1.87	0.56
1:B:241:LYS:HG2	6:B:2146:HOH:O	2.05	0.56
1:F:75:ASN:H	1:F:75:ASN:HD22	1.52	0.56
1:B:200:THR:HG22	1:B:225:VAL:HA	1.86	0.56
1:B:343:GLN:NE2	1:B:367:LYS:HD3	2.20	0.56
1:C:302:LEU:HD22	1:C:312:THR:HG21	1.87	0.56
1:C:494:VAL:CG1	1:C:518:LEU:HB2	2.36	0.56
1:F:200:THR:HG22	1:F:225:VAL:HA	1.87	0.56
1:A:80:HIS:H	1:A:98:ASN:HD21	1.51	0.56
1:B:456:ASN:ND2	1:B:456:ASN:H	2.02	0.56
1:F:80:HIS:H	1:F:98:ASN:HD21	1.51	0.56
1:A:337:THR:HB	1:A:374:PRO:HB2	1.87	0.56
1:B:56:GLY:O	1:B:60:THR:HG23	2.06	0.56
1:B:395:LEU:N	1:B:395:LEU:HD12	2.21	0.56
1:B:372:TYR:O	1:B:396:SER:HB3	2.05	0.56
1:E:266:PRO:HG2	6:E:2129:HOH:O	2.04	0.56
1:E:80:HIS:H	1:E:98:ASN:ND2	2.03	0.56
1:A:485:ASN:HB2	6:A:2289:HOH:O	2.04	0.56
1:B:492:THR:HG22	1:B:499:GLY:HA3	1.87	0.56
1:C:494:VAL:HG12	1:C:518:LEU:HB2	1.87	0.56
1:D:304:GLU:HB3	1:D:306:LYS:HG3	1.87	0.56
1:D:342:SER:HA	1:D:374:PRO:HD3	1.87	0.56
1:A:200:THR:HG22	1:A:225:VAL:HG22	1.86	0.56
1:A:304:GLU:HB3	1:A:306:LYS:HG3	1.87	0.56
1:C:53:SER:OG	1:D:75:ASN:HB2	2.06	0.56
1:A:15:GLY:HA2	1:B:402:ARG:NH2	2.21	0.56
1:C:366:GLN:NE2	1:C:424:MET:H	2.01	0.56
1:F:432:THR:HG21	1:F:436:PRO:HG3	1.87	0.56
1:B:261:ARG:HG2	1:B:302:LEU:HG	1.88	0.56
1:D:295:ALA:HB3	1:D:298:LYS:HD2	1.87	0.56
1:E:432:THR:HG21	1:E:436:PRO:HG3	1.86	0.55
1:E:472:VAL:HG12	1:E:479:LYS:HD2	1.88	0.55
1:E:523:ASP:OD1	1:F:410:HIS:HB2	2.07	0.55
1:B:456:ASN:HD22	1:B:456:ASN:N	2.04	0.55
1:E:449:THR:HG21	1:F:407:GLY:H	1.71	0.55
1:E:562:ASN:H	1:E:562:ASN:ND2	2.04	0.55
1:B:94:TYR:CD1	1:B:107:ARG:HD3	2.42	0.55
1:C:75:ASN:HD22	1:C:75:ASN:N	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:ALA:CB	1:B:496:PRO:CD	2.85	0.55
1:C:432:THR:HG21	1:C:436:PRO:HG3	1.88	0.55
1:F:559:TYR:CZ	1:F:574:GLY:HA3	2.42	0.55
1:A:61:ASN:HD21	1:A:548:THR:CG2	2.20	0.55
1:E:395:LEU:HD22	1:E:437:HIS:O	2.07	0.55
1:F:527:GLY:HA3	1:F:562:ASN:ND2	2.22	0.55
1:B:279:LYS:HB2	6:B:2156:HOH:O	2.07	0.55
1:A:559:TYR:CZ	1:A:574:GLY:HA3	2.42	0.55
1:B:337:THR:HB	1:B:374:PRO:HB2	1.89	0.55
1:C:18:ASP:HB3	1:C:37:VAL:O	2.06	0.55
1:A:181:VAL:HG21	1:A:231:ILE:HD13	1.89	0.54
1:A:494:VAL:CG1	1:A:518:LEU:HB2	2.38	0.54
1:D:79:HIS:H	1:D:98:ASN:ND2	2.06	0.54
1:A:512:THR:OG1	1:A:548:THR:HB	2.06	0.54
1:B:57:TRP:CH2	1:B:115:THR:HB	2.42	0.54
1:B:371:GLN:H	1:B:415:GLN:NE2	2.00	0.54
1:B:535:VAL:HG13	1:B:547:VAL:HG21	1.88	0.54
1:C:478:ASN:HD21	1:C:492:THR:HG22	1.71	0.54
1:D:266:PRO:HB2	1:D:288:SER:CB	2.38	0.54
1:A:344:VAL:HG23	1:A:370:VAL:CG2	2.33	0.54
1:F:392:LEU:HB2	1:F:419:ILE:HD13	1.88	0.54
1:A:186:ASN:ND2	1:A:205:ASN:H	2.05	0.54
1:A:267:LYS:HB3	1:A:287:LEU:HB2	1.87	0.54
1:A:395:LEU:HD22	1:A:437:HIS:O	2.08	0.54
1:C:470:ASP:HB3	1:C:481:ILE:CD1	2.37	0.54
1:D:37:VAL:HG21	1:D:441:LEU:HD22	1.89	0.54
1:F:61:ASN:ND2	6:F:2026:HOH:O	2.41	0.54
1:C:543:GLN:HG2	1:C:544:THR:N	2.21	0.54
1:D:188:ASP:HB3	1:D:202:THR:OG1	2.08	0.54
1:D:472:VAL:HG12	1:D:479:LYS:HD2	1.90	0.54
1:C:523:ASP:OD1	1:D:410:HIS:HB2	2.06	0.54
1:F:79:HIS:H	1:F:98:ASN:HD21	1.54	0.54
1:B:562:ASN:ND2	1:B:562:ASN:H	2.06	0.54
1:D:372:TYR:O	1:D:396:SER:HB3	2.07	0.54
1:F:412:GLU:HG3	1:F:436:PRO:HD2	1.90	0.54
1:F:528:PHE:O	1:F:536:SER:HA	2.08	0.54
1:A:158:PHE:O	1:B:575:ARG:NH2	2.41	0.54
1:A:29:GLN:HB2	1:A:434:ALA:HB3	1.90	0.53
1:C:25:SER:HB3	1:C:81:PRO:HD3	1.90	0.53
1:D:302:LEU:HD22	1:D:312:THR:HG21	1.90	0.53
1:A:371:GLN:N	1:A:415:GLN:HE22	1.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:LYS:HB3	1:D:287:LEU:HB2	1.89	0.53
1:F:371:GLN:H	1:F:415:GLN:NE2	1.99	0.53
1:B:48:VAL:H	1:B:50:ASN:HD21	1.55	0.53
1:B:78:CYS:HB2	1:B:97:ILE:CD1	2.38	0.53
1:D:538:GLU:C	1:D:539:ILE:HG13	2.28	0.53
1:E:371:GLN:HG2	1:E:402:ARG:CZ	2.38	0.53
1:F:227:ASN:O	1:F:231:ILE:HG13	2.08	0.53
1:A:302:LEU:HD22	1:A:312:THR:HG21	1.90	0.53
1:C:395:LEU:HD12	1:C:395:LEU:H	1.73	0.53
1:E:20:TYR:HB2	1:E:37:VAL:HB	1.89	0.53
1:C:339:PHE:CE1	1:C:373:GLN:HB3	2.44	0.53
1:D:35:LEU:HD23	1:D:42:GLU:HA	1.91	0.53
1:B:304:GLU:HB3	1:B:306:LYS:HG3	1.88	0.53
1:B:415:GLN:HB3	1:B:426:LEU:HD11	1.89	0.53
1:B:494:VAL:CG1	1:B:518:LEU:HB2	2.39	0.53
1:C:263:ILE:O	1:C:265:VAL:HG23	2.09	0.53
1:F:144:ASN:HB3	1:F:187:LEU:HB3	1.91	0.53
1:A:478:ASN:HD21	1:A:492:THR:CG2	2.20	0.53
1:D:528:PHE:O	1:D:536:SER:HA	2.08	0.53
1:F:124:VAL:HG13	1:F:125:GLN:N	2.22	0.53
1:A:456:ASN:H	1:A:456:ASN:HD22	1.57	0.53
1:B:75:ASN:H	1:B:75:ASN:HD22	1.57	0.53
1:E:527:GLY:HA3	1:E:562:ASN:HD21	1.73	0.53
1:F:342:SER:HA	1:F:374:PRO:HD3	1.91	0.53
1:B:452:ILE:HD13	1:B:542:GLN:HG3	1.91	0.53
1:B:28:HIS:HA	1:B:77:ASP:HA	1.91	0.53
1:D:562:ASN:HD22	1:D:562:ASN:N	2.05	0.53
1:E:467:ALA:HB1	1:E:472:VAL:HG23	1.91	0.53
1:E:406:VAL:O	1:F:113:MET:HG3	2.09	0.53
1:C:495:ALA:CB	1:C:496:PRO:HD2	2.37	0.53
1:B:29:GLN:HB2	1:B:434:ALA:HB3	1.91	0.52
1:D:286:LYS:N	1:D:323:PRO:HG2	2.24	0.52
1:D:29:GLN:HB2	1:D:434:ALA:HB3	1.90	0.52
1:D:50:ASN:ND2	1:D:50:ASN:H	2.07	0.52
1:E:48:VAL:H	1:E:50:ASN:HD21	1.57	0.52
1:C:534:GLY:HA2	1:D:75:ASN:ND2	2.24	0.52
1:D:343:GLN:HA	1:D:370:VAL:HG23	1.90	0.52
1:D:517:ASN:HB2	1:D:539:ILE:HG22	1.92	0.52
1:D:339:PHE:HA	1:D:374:PRO:HD2	1.92	0.52
1:F:79:HIS:H	1:F:98:ASN:ND2	2.07	0.52
1:C:296:ILE:HG23	1:C:299:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:H	1:A:75:ASN:HD22	1.55	0.52
1:B:302:LEU:HD22	1:B:312:THR:HG21	1.91	0.52
1:B:343:GLN:HE22	1:B:367:LYS:HD3	1.75	0.52
1:D:202:THR:HG23	1:D:272:LEU:HB2	1.92	0.52
1:D:494:VAL:HG13	1:D:518:LEU:HB2	1.92	0.52
1:D:494:VAL:CG1	1:D:518:LEU:HB2	2.39	0.52
1:F:454:GLU:HB3	6:F:2156:HOH:O	2.10	0.52
1:E:534:GLY:HA2	1:F:75:ASN:ND2	2.23	0.52
1:A:412:GLU:HG3	1:A:436:PRO:HD2	1.92	0.52
1:B:371:GLN:HG2	1:B:402:ARG:HD2	1.92	0.52
1:D:117:LYS:HB2	1:D:175:MET:HG3	1.91	0.52
1:D:495:ALA:CB	1:D:496:PRO:HD2	2.37	0.52
1:E:231:ILE:O	1:E:235:VAL:HG23	2.09	0.52
1:A:443:ARG:H	1:A:446:GLN:NE2	2.02	0.52
1:D:18:ASP:HB3	1:D:37:VAL:O	2.09	0.52
1:E:344:VAL:HG23	1:E:370:VAL:CG2	2.38	0.52
1:E:372:TYR:O	1:E:396:SER:HB3	2.10	0.52
1:C:93:LYS:HE2	1:C:94:TYR:CZ	2.44	0.51
1:F:83:ILE:HG22	1:F:440:ILE:HD13	1.91	0.51
1:A:202:THR:HG23	1:A:272:LEU:HB2	1.93	0.51
1:C:372:TYR:O	1:C:396:SER:HB3	2.11	0.51
1:E:158:PHE:O	1:F:575:ARG:NH2	2.43	0.51
1:E:295:ALA:HB2	1:E:314:VAL:HG21	1.92	0.51
1:A:443:ARG:N	1:A:446:GLN:HE21	2.02	0.51
1:B:373:GLN:HE21	1:B:398:PHE:HD2	1.57	0.51
1:B:390:LYS:HG2	6:B:2010:HOH:O	2.09	0.51
1:C:495:ALA:CB	1:C:496:PRO:CD	2.86	0.51
1:E:517:ASN:HB2	1:E:539:ILE:HG22	1.91	0.51
1:F:261:ARG:CZ	1:F:303:PHE:HA	2.40	0.51
1:C:50:ASN:H	1:C:50:ASN:ND2	2.06	0.51
1:E:528:PHE:O	1:E:536:SER:HA	2.10	0.51
1:B:186:ASN:HD21	1:B:204:TYR:H	1.59	0.51
1:A:495:ALA:CB	1:A:496:PRO:HD2	2.39	0.51
1:D:186:ASN:HD22	1:D:186:ASN:N	2.09	0.51
1:D:186:ASN:ND2	1:D:205:ASN:H	2.09	0.51
1:D:80:HIS:H	1:D:98:ASN:ND2	2.08	0.51
1:E:407:GLY:H	1:F:449:THR:HG21	1.76	0.51
1:F:295:ALA:HB2	1:F:314:VAL:HG21	1.93	0.51
1:A:291:VAL:O	1:A:316:GLU:HA	2.11	0.51
1:E:325:HIS:CE1	1:E:376:HIS:CE1	2.99	0.51
1:E:18:ASP:HB3	1:E:37:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:566:HIS:HB2	6:E:2222:HOH:O	2.11	0.51
1:A:339:PHE:CE1	1:A:373:GLN:HB3	2.46	0.51
1:A:535:VAL:HG13	1:A:547:VAL:HG21	1.92	0.51
1:B:432:THR:HG21	1:B:436:PRO:HG3	1.92	0.51
1:C:231:ILE:O	1:C:235:VAL:HG23	2.10	0.51
1:C:78:CYS:HA	1:C:98:ASN:O	2.11	0.51
1:C:125:GLN:HE22	1:D:558:TRP:H	1.57	0.51
1:F:152:PRO:HG2	1:F:154:ASP:OD2	2.11	0.51
1:F:29:GLN:HB2	1:F:434:ALA:CB	2.40	0.51
1:D:279:LYS:HB2	6:D:2054:HOH:O	2.10	0.51
1:A:261:ARG:HG2	1:A:302:LEU:HG	1.92	0.50
1:C:78:CYS:HB2	1:C:97:ILE:CD1	2.41	0.50
1:D:109:ARG:NH2	1:D:112:ILE:HD13	2.26	0.50
1:D:90:TYR:CD2	1:D:442:VAL:HG12	2.46	0.50
1:E:53:SER:OG	1:F:75:ASN:HB2	2.11	0.50
1:E:78:CYS:HB2	1:E:97:ILE:CD1	2.42	0.50
1:A:495:ALA:HB3	6:A:2294:HOH:O	2.11	0.50
1:B:29:GLN:HB2	1:B:434:ALA:HB1	1.93	0.50
1:B:80:HIS:H	1:B:98:ASN:HD21	1.60	0.50
1:C:37:VAL:HG21	1:C:441:LEU:HD22	1.92	0.50
1:C:478:ASN:HD21	1:C:492:THR:CG2	2.23	0.50
1:C:404:LEU:HD11	1:D:18:ASP:HB2	1.93	0.50
1:F:96:PHE:CE2	1:F:107:ARG:HG3	2.46	0.50
1:B:25:SER:HB3	1:B:81:PRO:HD3	1.93	0.50
1:A:564:PHE:HB2	1:B:435:GLU:OE2	2.12	0.50
1:C:78:CYS:HB2	1:C:97:ILE:HG12	1.93	0.50
1:E:109:ARG:HH21	1:E:112:ILE:CD1	2.24	0.50
1:E:109:ARG:HH21	1:E:112:ILE:HD13	1.76	0.50
1:E:75:ASN:HD22	1:E:75:ASN:H	1.58	0.50
1:F:186:ASN:ND2	1:F:205:ASN:H	2.10	0.50
1:F:470:ASP:HB3	1:F:481:ILE:CD1	2.41	0.50
1:A:485:ASN:HB3	6:A:2302:HOH:O	2.11	0.50
1:A:527:GLY:HA3	1:A:562:ASN:ND2	2.27	0.50
1:A:57:TRP:CH2	1:A:115:THR:HB	2.46	0.50
1:E:21:TYR:HB2	1:E:442:VAL:CG2	2.42	0.50
1:F:277:ASP:OD1	1:F:279:LYS:HG2	2.10	0.50
1:F:344:VAL:HG21	1:F:394:VAL:HG21	1.94	0.50
1:F:50:ASN:H	1:F:50:ASN:ND2	2.03	0.50
1:F:57:TRP:CH2	1:F:115:THR:HB	2.47	0.50
1:A:45:ARG:NH2	6:A:2013:HOH:O	2.25	0.50
1:B:125:GLN:HG3	1:B:149:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:THR:O	1:E:261:ARG:HD2	2.12	0.50
1:A:37:VAL:HG21	1:A:441:LEU:HD22	1.94	0.50
1:D:186:ASN:HD21	1:D:205:ASN:H	1.59	0.50
1:E:548:THR:HG21	6:E:2012:HOH:O	2.10	0.50
1:F:261:ARG:HG2	1:F:302:LEU:HG	1.94	0.50
1:F:343:GLN:HE21	1:F:367:LYS:HD3	1.75	0.50
1:F:371:GLN:N	1:F:415:GLN:HE22	1.99	0.50
1:F:530:MET:SD	1:F:559:TYR:HB3	2.52	0.50
1:A:279:LYS:HB2	6:A:2178:HOH:O	2.11	0.50
1:B:339:PHE:CE1	1:B:373:GLN:HB3	2.47	0.50
1:C:200:THR:CG2	1:C:225:VAL:HG22	2.42	0.50
1:D:165:THR:HG21	1:D:186:ASN:HA	1.93	0.50
1:D:288:SER:C	1:D:290:THR:H	2.15	0.50
1:A:449:THR:HB	6:A:2262:HOH:O	2.12	0.49
1:D:553:LYS:HG3	6:D:2110:HOH:O	2.12	0.49
1:E:107:ARG:NH1	1:E:116:ASP:OD2	2.43	0.49
1:E:543:GLN:HG2	1:E:544:THR:N	2.27	0.49
1:C:339:PHE:HA	1:C:374:PRO:HD2	1.94	0.49
1:D:29:GLN:HB2	1:D:434:ALA:CB	2.41	0.49
1:D:343:GLN:NE2	1:D:367:LYS:HD3	2.27	0.49
1:D:376:HIS:HB2	1:D:437:HIS:O	2.11	0.49
1:A:343:GLN:NE2	1:A:367:LYS:HD3	2.27	0.49
1:F:281:PHE:CD2	1:F:296:ILE:HG12	2.47	0.49
1:F:75:ASN:N	1:F:75:ASN:HD22	2.09	0.49
1:C:322:GLY:N	1:C:323:PRO:HD3	2.27	0.49
1:A:227:ASN:O	1:A:231:ILE:HG13	2.12	0.49
1:B:202:THR:HG23	1:B:272:LEU:HD12	1.94	0.49
1:B:282:ILE:HG23	1:B:291:VAL:HG13	1.93	0.49
1:B:495:ALA:O	6:B:2265:HOH:O	2.19	0.49
1:A:212:LEU:HD12	1:B:497:GLN:OE1	2.13	0.49
1:B:538:GLU:C	1:B:539:ILE:HG13	2.33	0.49
1:C:35:LEU:HD23	1:C:42:GLU:HA	1.94	0.49
1:F:540:SER:HB3	1:F:541:PRO:HD2	1.95	0.49
1:C:29:GLN:HB2	1:C:434:ALA:HB3	1.93	0.49
1:D:21:TYR:HB2	1:D:442:VAL:CG2	2.43	0.49
1:E:80:HIS:H	1:E:98:ASN:HD21	1.59	0.49
1:F:35:LEU:CD2	1:F:42:GLU:HA	2.43	0.49
1:B:210:VAL:HG12	6:B:2133:HOH:O	2.13	0.49
1:B:540:SER:HB3	1:B:541:PRO:CD	2.43	0.49
1:C:343:GLN:NE2	1:C:367:LYS:HD3	2.27	0.49
1:C:528:PHE:O	1:C:536:SER:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:TYR:CD1	1:E:107:ARG:HD3	2.47	0.49
1:A:371:GLN:HG2	1:A:402:ARG:HD2	1.96	0.48
1:C:197:LYS:HG3	1:C:229:GLU:HB2	1.95	0.48
1:E:494:VAL:CG1	1:E:518:LEU:HB2	2.43	0.48
1:F:50:ASN:N	1:F:50:ASN:HD22	2.02	0.48
1:A:411:PRO:HB3	1:B:43:LEU:O	2.13	0.48
1:E:217:ARG:HD2	6:E:2095:HOH:O	2.13	0.48
1:F:495:ALA:CB	1:F:496:PRO:HD2	2.43	0.48
1:A:197:LYS:HG3	1:A:229:GLU:HB2	1.95	0.48
1:B:575:ARG:HD3	6:B:2274:HOH:O	2.12	0.48
1:B:75:ASN:N	1:B:75:ASN:HD22	2.10	0.48
1:D:191:ASP:OD1	1:D:192:ALA:N	2.45	0.48
1:D:261:ARG:HG2	1:D:302:LEU:HG	1.95	0.48
1:E:125:GLN:HE22	1:F:558:TRP:H	1.61	0.48
1:E:200:THR:CG2	1:E:225:VAL:HG22	2.43	0.48
1:F:343:GLN:HB3	1:F:369:ASP:HA	1.94	0.48
1:B:223:VAL:HG23	1:B:265:VAL:HG21	1.95	0.48
1:C:35:LEU:CD2	1:C:42:GLU:HA	2.43	0.48
1:D:543:GLN:HG2	1:D:544:THR:N	2.29	0.48
1:D:85:MET:CE	1:D:134:LYS:HG2	2.43	0.48
1:B:371:GLN:HG2	1:B:402:ARG:NH1	2.29	0.48
1:C:21:TYR:HB2	1:C:442:VAL:CG2	2.44	0.48
1:C:449:THR:HG21	1:D:407:GLY:H	1.77	0.48
1:D:296:ILE:HG23	1:D:299:LEU:HD12	1.95	0.48
1:A:407:GLY:N	1:B:449:THR:HG21	2.28	0.48
1:A:538:GLU:HB2	1:A:563:TRP:CH2	2.48	0.48
1:B:47:PRO:HA	1:B:50:ASN:HD21	1.78	0.48
1:B:559:TYR:CZ	1:B:574:GLY:HA3	2.49	0.48
1:E:46:ILE:HG21	1:E:108:ILE:HD13	1.94	0.48
1:E:135:VAL:HG13	1:E:136:PRO:HA	1.94	0.48
1:E:491:MET:HB2	1:E:515:ILE:CD1	2.43	0.48
1:E:61:ASN:HD21	1:E:548:THR:CG2	2.26	0.48
1:E:78:CYS:HA	1:E:98:ASN:O	2.14	0.48
1:F:135:VAL:HG13	1:F:136:PRO:HA	1.94	0.48
1:C:47:PRO:HA	1:C:50:ASN:HD21	1.77	0.48
1:D:295:ALA:HB2	1:D:314:VAL:HG21	1.94	0.48
1:E:109:ARG:HG3	1:E:116:ASP:HB2	1.95	0.48
1:A:301:ASP:OD1	1:A:306:LYS:HD2	2.12	0.48
1:B:467:ALA:HB1	1:B:472:VAL:HG22	1.96	0.48
1:B:98:ASN:H	1:B:98:ASN:HD22	1.60	0.48
1:E:109:ARG:NH2	1:E:112:ILE:HD13	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:GLN:H	1:E:415:GLN:NE2	1.94	0.48
1:B:491:MET:HB2	1:B:515:ILE:HD13	1.96	0.48
1:C:449:THR:HG22	1:C:450:LYS:N	2.29	0.48
1:E:83:ILE:HG22	1:E:440:ILE:HD13	1.95	0.48
1:F:329:ASP:OD2	1:F:333:ASN:HB2	2.14	0.48
1:A:370:VAL:HG13	1:A:415:GLN:NE2	2.29	0.48
1:D:78:CYS:HA	1:D:98:ASN:O	2.14	0.48
1:F:456:ASN:C	1:F:456:ASN:HD22	2.16	0.48
1:A:323:PRO:HA	1:A:337:THR:O	2.14	0.47
1:B:449:THR:HG21	6:B:2230:HOH:O	2.14	0.47
1:D:133:GLN:OE1	1:D:139:ASN:HB2	2.14	0.47
1:D:366:GLN:HE22	1:D:423:GLU:HA	1.79	0.47
1:F:282:ILE:HG23	1:F:291:VAL:CG1	2.42	0.47
1:F:18:ASP:HB3	1:F:37:VAL:O	2.14	0.47
1:C:540:SER:HB3	1:C:541:PRO:CD	2.44	0.47
1:C:291:VAL:O	1:C:316:GLU:HA	2.15	0.47
1:D:321:LEU:HD12	1:D:341:ASP:OD1	2.14	0.47
1:D:562:ASN:N	1:D:562:ASN:ND2	2.59	0.47
1:D:75:ASN:H	1:D:75:ASN:HD22	1.61	0.47
1:A:202:THR:HG23	1:A:272:LEU:HD12	1.95	0.47
1:A:29:GLN:HB2	1:A:434:ALA:CB	2.43	0.47
1:A:78:CYS:HA	1:A:98:ASN:O	2.14	0.47
1:C:456:ASN:N	1:C:456:ASN:HD22	2.08	0.47
1:E:220:ARG:HD2	6:E:2100:HOH:O	2.13	0.47
1:E:443:ARG:N	1:E:446:GLN:HE21	1.92	0.47
1:F:202:THR:HG23	1:F:272:LEU:HD12	1.95	0.47
1:A:286:LYS:NZ	6:A:2179:HOH:O	2.47	0.47
1:C:284:ASN:ND2	1:C:325:HIS:HA	2.30	0.47
1:C:547:VAL:HG13	1:C:547:VAL:O	2.14	0.47
1:C:80:HIS:H	1:C:98:ASN:HD21	1.62	0.47
1:D:82:HIS:NE2	1:D:131:ARG:HG2	2.30	0.47
1:D:366:GLN:HG2	1:D:367:LYS:N	2.30	0.47
1:F:72:GLN:HG3	6:F:2035:HOH:O	2.13	0.47
1:B:186:ASN:HD22	1:B:186:ASN:H	1.62	0.47
1:A:287:LEU:HD21	1:B:568:LEU:HD21	1.97	0.47
1:C:130:LEU:HD23	1:C:130:LEU:C	2.35	0.47
1:C:304:GLU:HG2	1:C:306:LYS:HE2	1.97	0.47
1:C:212:LEU:HD11	1:D:496:PRO:HG2	1.96	0.47
1:F:449:THR:CG2	1:F:450:LYS:N	2.78	0.47
1:B:193:ASP:HB2	6:B:2125:HOH:O	2.13	0.47
1:D:207:GLU:HG3	1:D:218:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:GLN:HG3	1:D:33:ARG:HH21	1.79	0.47
1:E:295:ALA:HB2	1:E:314:VAL:CG2	2.43	0.47
1:E:403:PHE:HB3	1:F:43:LEU:HD22	1.97	0.47
1:A:174:THR:HG21	6:A:2109:HOH:O	2.14	0.47
1:B:302:LEU:HD11	1:B:309:LEU:HD23	1.96	0.47
1:E:494:VAL:HA	6:E:2213:HOH:O	2.15	0.47
1:F:11:HIS:HB3	6:F:2003:HOH:O	2.15	0.47
1:B:527:GLY:HA3	1:B:562:ASN:HD21	1.78	0.47
1:D:547:VAL:HG13	1:D:547:VAL:O	2.15	0.47
1:E:530:MET:SD	1:E:559:TYR:HB3	2.55	0.47
1:B:467:ALA:HB1	1:B:472:VAL:CG2	2.45	0.47
1:D:327:THR:HG22	1:D:335:TYR:HB2	1.97	0.47
1:D:344:VAL:HG21	1:D:394:VAL:HG21	1.96	0.47
1:F:144:ASN:HB3	1:F:187:LEU:CB	2.45	0.47
1:C:288:SER:C	1:C:290:THR:H	2.18	0.47
1:D:186:ASN:HD21	1:D:204:TYR:H	1.63	0.47
1:E:537:MET:HE2	1:E:547:VAL:HG12	1.95	0.47
1:C:515:ILE:HG21	1:C:539:ILE:HD13	1.96	0.46
1:F:265:VAL:HG13	1:F:292:SER:OG	2.16	0.46
1:F:494:VAL:CG1	1:F:518:LEU:HB2	2.44	0.46
1:A:339:PHE:HA	1:A:374:PRO:HD2	1.97	0.46
1:C:397:LYS:HE2	6:C:2055:HOH:O	2.15	0.46
1:D:231:ILE:O	1:D:235:VAL:HG23	2.15	0.46
1:D:327:THR:HG22	1:D:377:ASN:ND2	2.30	0.46
1:D:456:ASN:H	1:D:456:ASN:HD22	1.62	0.46
1:D:57:TRP:CH2	1:D:115:THR:HB	2.50	0.46
1:A:75:ASN:HD22	1:A:75:ASN:N	2.12	0.46
1:B:470:ASP:CB	1:B:481:ILE:HD13	2.40	0.46
1:B:540:SER:H	1:B:543:GLN:NE2	2.13	0.46
1:D:450:LYS:HD3	6:D:2069:HOH:O	2.15	0.46
1:D:452:ILE:HG13	1:D:452:ILE:O	2.15	0.46
1:D:559:TYR:CE1	1:D:574:GLY:HA3	2.50	0.46
1:A:541:PRO:O	1:A:542:GLN:HB2	2.15	0.46
1:B:538:GLU:HG2	1:B:539:ILE:N	2.31	0.46
1:C:411:PRO:HB3	1:D:43:LEU:O	2.15	0.46
1:E:304:GLU:HB3	1:E:306:LYS:HG3	1.97	0.46
1:A:95:LEU:HD23	1:A:96:PHE:N	2.30	0.46
1:B:231:ILE:O	1:B:235:VAL:HG23	2.15	0.46
1:E:186:ASN:ND2	1:E:205:ASN:H	2.14	0.46
1:F:223:VAL:HG23	1:F:265:VAL:HG21	1.98	0.46
1:B:366:GLN:HG2	1:B:367:LYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:ILE:HG21	1:B:539:ILE:HD13	1.97	0.46
1:C:117:LYS:HB2	1:C:175:MET:HG3	1.98	0.46
1:D:469:LYS:HD3	6:D:2081:HOH:O	2.15	0.46
1:D:78:CYS:HB2	1:D:97:ILE:HG12	1.98	0.46
1:F:143:CYS:SG	1:F:168:THR:HB	2.56	0.46
1:A:329:ASP:OD2	1:A:333:ASN:HB2	2.16	0.46
1:A:521:VAL:HG23	6:A:2307:HOH:O	2.16	0.46
1:B:37:VAL:HG13	1:B:38:PRO:HA	1.97	0.46
1:D:37:VAL:HG13	1:D:38:PRO:HA	1.98	0.46
1:A:61:ASN:HD21	1:A:548:THR:HG23	1.80	0.46
1:C:337:THR:HB	1:C:374:PRO:HB2	1.98	0.46
1:C:67:LEU:HD23	1:C:118:ILE:HD13	1.97	0.46
1:A:245:ASP:HB3	1:F:156:THR:HB	1.98	0.46
1:C:562:ASN:ND2	1:C:562:ASN:H	2.14	0.46
1:F:284:ASN:ND2	1:F:325:HIS:HA	2.31	0.46
1:A:288:SER:C	1:A:290:THR:H	2.19	0.45
1:A:376:HIS:HB2	1:A:437:HIS:O	2.15	0.45
1:B:296:ILE:HG23	1:B:299:LEU:HD12	1.98	0.45
1:B:338:LEU:HD12	1:B:343:GLN:HE21	1.80	0.45
1:C:407:GLY:H	1:D:449:THR:CG2	2.29	0.45
1:E:464:ARG:HD3	6:E:2198:HOH:O	2.16	0.45
1:F:372:TYR:CD1	1:F:400:LYS:HD2	2.50	0.45
1:F:366:GLN:NE2	1:F:424:MET:H	2.11	0.45
1:F:49:PHE:CZ	1:F:99:ASP:HB2	2.51	0.45
1:C:142:PHE:HB3	1:C:167:PHE:CZ	2.51	0.45
1:C:266:PRO:HB2	6:C:2050:HOH:O	2.15	0.45
1:C:376:HIS:CE1	1:C:438:ASP:HB2	2.51	0.45
1:D:360:ARG:HB2	1:D:360:ARG:HE	1.51	0.45
1:E:181:VAL:HG21	1:E:231:ILE:HD13	1.97	0.45
1:B:535:VAL:CG1	1:B:547:VAL:HG11	2.46	0.45
1:C:390:LYS:HG2	6:C:2003:HOH:O	2.15	0.45
1:F:117:LYS:HB2	1:F:175:MET:HG3	1.96	0.45
1:F:495:ALA:HA	6:F:2182:HOH:O	2.16	0.45
1:F:540:SER:HB3	1:F:541:PRO:CD	2.46	0.45
1:F:535:VAL:HG13	1:F:547:VAL:HG21	1.97	0.45
1:A:342:SER:HA	1:A:374:PRO:HD3	1.97	0.45
1:B:540:SER:HB3	1:B:541:PRO:HD2	1.99	0.45
1:D:291:VAL:O	1:D:316:GLU:HA	2.16	0.45
1:C:75:ASN:ND2	1:D:534:GLY:HA2	2.22	0.45
1:D:28:HIS:HA	1:D:77:ASP:HA	1.98	0.45
1:A:530:MET:SD	1:A:559:TYR:HB3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:HIS:H	1:A:98:ASN:ND2	2.13	0.45
1:B:265:VAL:HG13	1:B:266:PRO:HD2	1.98	0.45
1:D:361:VAL:HG12	1:D:362:ASN:N	2.32	0.45
1:E:29:GLN:HB2	1:E:434:ALA:HB3	1.98	0.45
1:E:547:VAL:O	1:E:547:VAL:HG13	2.17	0.45
1:B:328:PHE:N	1:B:328:PHE:CD1	2.85	0.45
1:C:221:ASP:O	1:C:264:PRO:HA	2.17	0.45
1:D:61:ASN:OD1	1:D:548:THR:HG22	2.16	0.45
1:D:575:ARG:HD3	6:D:2095:HOH:O	2.16	0.45
1:E:286:LYS:HD3	6:E:2125:HOH:O	2.17	0.45
1:F:221:ASP:O	1:F:264:PRO:HA	2.17	0.45
1:F:456:ASN:ND2	6:F:2156:HOH:O	2.49	0.45
1:A:188:ASP:HB3	1:A:202:THR:OG1	2.16	0.45
1:C:189:ASN:O	1:C:201:SER:HA	2.17	0.45
1:D:343:GLN:HB3	1:D:369:ASP:HA	1.99	0.45
1:E:562:ASN:HD22	1:E:562:ASN:H	1.65	0.45
1:F:29:GLN:HB2	1:F:434:ALA:HB3	1.99	0.45
1:B:349:ILE:HB	6:B:2178:HOH:O	2.17	0.45
1:E:105:VAL:HG21	1:E:143:CYS:SG	2.57	0.45
1:E:179:TRP:CZ3	1:E:231:ILE:HG21	2.52	0.45
1:E:321:LEU:HB3	1:E:340:ILE:HB	1.98	0.45
1:F:449:THR:HG22	1:F:450:LYS:N	2.32	0.45
1:F:538:GLU:HB2	1:F:563:TRP:CH2	2.51	0.45
1:A:133:GLN:OE1	1:A:139:ASN:HB2	2.17	0.45
1:A:373:GLN:HE21	1:A:398:PHE:HD2	1.65	0.45
1:B:562:ASN:HD22	1:B:562:ASN:H	1.64	0.45
1:C:151:GLN:HA	1:C:152:PRO:HA	1.85	0.45
1:C:165:THR:HG21	1:C:186:ASN:HA	1.99	0.45
1:C:210:VAL:HG12	6:C:2038:HOH:O	2.17	0.45
1:C:319:LEU:HD22	1:C:345:CYS:SG	2.56	0.45
1:F:142:PHE:HB3	1:F:167:PHE:CZ	2.52	0.45
1:F:83:ILE:CD1	1:F:92:GLY:HA2	2.28	0.45
1:A:371:GLN:HG2	1:A:402:ARG:CZ	2.46	0.45
1:B:286:LYS:H	1:B:323:PRO:HG2	1.82	0.45
1:C:193:ASP:OD2	1:C:198:TYR:HB2	2.17	0.45
1:C:262:TYR:O	1:C:264:PRO:HD3	2.17	0.45
1:E:200:THR:HG22	1:E:225:VAL:HG22	1.98	0.45
1:E:456:ASN:HD22	1:E:456:ASN:N	2.05	0.45
1:F:342:SER:HA	1:F:374:PRO:CD	2.47	0.45
1:F:495:ALA:HB3	6:F:2184:HOH:O	2.16	0.45
1:A:135:VAL:HG13	1:A:136:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ASP:OD1	1:B:410:HIS:HB2	2.17	0.44
1:C:268:ASN:O	1:C:286:LYS:HE2	2.17	0.44
1:D:521:VAL:HB	1:D:524:VAL:HG21	1.98	0.44
1:E:133:GLN:OE1	1:E:139:ASN:HB2	2.16	0.44
1:E:202:THR:HG23	1:E:272:LEU:HD12	1.98	0.44
1:E:47:PRO:HA	1:E:50:ASN:HD21	1.82	0.44
1:A:304:GLU:HG2	1:A:306:LYS:HE2	1.99	0.44
1:C:381:LEU:HB2	1:C:387:ALA:HA	2.00	0.44
1:E:505:VAL:O	1:E:578:VAL:HA	2.16	0.44
1:F:495:ALA:C	6:F:2182:HOH:O	2.55	0.44
1:F:495:ALA:HB1	1:F:496:PRO:HD3	1.96	0.44
1:F:540:SER:H	1:F:543:GLN:HE21	1.62	0.44
1:A:433:TYR:CG	1:A:434:ALA:N	2.86	0.44
1:A:456:ASN:N	1:A:456:ASN:HD22	2.14	0.44
1:B:134:LYS:HE3	6:B:2088:HOH:O	2.16	0.44
1:B:432:THR:HG22	1:B:433:TYR:N	2.33	0.44
1:B:433:TYR:CG	1:B:434:ALA:N	2.85	0.44
1:C:343:GLN:HA	1:C:370:VAL:H	1.82	0.44
1:E:286:LYS:NZ	6:E:2125:HOH:O	2.51	0.44
1:F:262:TYR:O	1:F:264:PRO:HD3	2.17	0.44
1:A:247:LYS:HE3	6:F:2063:HOH:O	2.17	0.44
1:B:495:ALA:CA	6:B:2265:HOH:O	2.65	0.44
1:D:131:ARG:HD2	1:D:191:ASP:CG	2.38	0.44
1:D:223:VAL:HG23	1:D:265:VAL:HG21	1.99	0.44
1:F:302:LEU:HD11	1:F:309:LEU:HD23	1.99	0.44
1:F:323:PRO:HA	1:F:337:THR:O	2.17	0.44
1:B:370:VAL:HG13	1:B:415:GLN:NE2	2.31	0.44
1:A:435:GLU:OE2	1:B:564:PHE:HB2	2.17	0.44
1:C:61:ASN:ND2	1:C:548:THR:HG22	2.30	0.44
1:E:320:GLY:HA3	1:E:338:LEU:HD13	1.98	0.44
1:B:495:ALA:CB	1:B:496:PRO:HD2	2.47	0.44
1:B:511:VAL:O	1:B:548:THR:HA	2.18	0.44
1:C:276:PRO:HD3	1:C:328:PHE:CG	2.53	0.44
1:E:531:VAL:HG11	1:F:125:GLN:HG2	1.99	0.44
1:A:95:LEU:HB2	1:A:110:LEU:HD21	2.00	0.44
1:A:160:LEU:HD11	1:A:210:VAL:HG12	1.99	0.44
1:B:370:VAL:HG13	6:B:2212:HOH:O	2.18	0.44
1:B:371:GLN:CB	1:B:402:ARG:HD2	2.48	0.44
1:C:29:GLN:HB2	1:C:434:ALA:CB	2.48	0.44
1:C:457:ASP:HA	1:C:458:PRO:HD3	1.88	0.44
1:C:28:HIS:HA	1:C:77:ASP:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:SER:O	1:D:40:MET:HB2	2.16	0.44
1:E:553:LYS:HB2	1:E:554:PRO:HD2	2.00	0.44
1:A:147:PHE:HB3	1:B:558:TRP:CE2	2.52	0.44
1:B:395:LEU:H	1:B:395:LEU:HD12	1.83	0.44
1:C:491:MET:HB2	1:C:515:ILE:CD1	2.46	0.44
1:E:202:THR:HG23	1:E:272:LEU:HB2	2.00	0.44
1:E:276:PRO:HD3	1:E:328:PHE:CG	2.53	0.44
1:A:433:TYR:CE2	1:A:434:ALA:HB2	2.53	0.43
1:A:75:ASN:ND2	1:A:102:ASN:HD21	2.16	0.43
1:B:207:GLU:HG3	1:B:218:ASN:ND2	2.33	0.43
1:C:210:VAL:HG13	1:C:211:ASP:N	2.33	0.43
1:F:529:CYS:O	1:F:559:TYR:HA	2.17	0.43
1:B:212:LEU:HD22	1:B:216:MET:SD	2.58	0.43
1:B:360:ARG:HB2	1:B:360:ARG:HE	1.69	0.43
1:B:540:SER:H	1:B:543:GLN:HE21	1.66	0.43
1:C:395:LEU:N	1:C:395:LEU:HD12	2.33	0.43
1:C:49:PHE:CE2	1:C:99:ASP:HB2	2.53	0.43
1:D:538:GLU:HG2	1:D:539:ILE:N	2.32	0.43
1:E:496:PRO:HG3	1:E:568:LEU:HB2	2.00	0.43
1:F:281:PHE:CE2	1:F:296:ILE:HG12	2.53	0.43
1:F:390:LYS:HE3	1:F:420:SER:HB2	2.00	0.43
1:A:130:LEU:C	1:A:130:LEU:HD23	2.39	0.43
1:B:449:THR:HG22	1:B:450:LYS:N	2.33	0.43
1:B:78:CYS:HA	1:B:98:ASN:O	2.17	0.43
1:E:38:PRO:HD3	6:E:2169:HOH:O	2.18	0.43
1:E:82:HIS:O	1:E:95:LEU:HA	2.19	0.43
1:F:266:PRO:HB2	1:F:288:SER:HB2	2.00	0.43
1:F:290:THR:HG22	1:F:318:GLU:CA	2.48	0.43
1:F:433:TYR:CG	1:F:434:ALA:N	2.86	0.43
1:B:481:ILE:HD12	1:B:490:TYR:CE1	2.52	0.43
1:C:61:ASN:HD21	1:C:548:THR:HG21	1.81	0.43
1:C:75:ASN:HB2	1:D:53:SER:OG	2.18	0.43
1:D:109:ARG:NH2	1:D:112:ILE:CD1	2.81	0.43
1:D:363:TYR:CD1	1:D:364:ILE:HG13	2.54	0.43
1:D:454:GLU:HG3	6:D:2069:HOH:O	2.19	0.43
1:D:515:ILE:HG21	1:D:539:ILE:HD13	2.00	0.43
1:E:67:LEU:HD23	1:E:118:ILE:HD13	1.99	0.43
1:F:109:ARG:HB3	1:F:111:ASP:OD1	2.19	0.43
1:A:166:MET:HG2	1:A:182:ILE:HA	1.99	0.43
1:C:188:ASP:HB3	1:C:202:THR:OG1	2.19	0.43
1:D:365:ARG:HH11	1:D:365:ARG:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:302:LEU:HD22	1:E:312:THR:HG21	1.99	0.43
1:E:61:ASN:HD21	1:E:548:THR:HG22	1.83	0.43
1:F:366:GLN:HG2	1:F:367:LYS:N	2.34	0.43
1:A:83:ILE:HG22	1:A:440:ILE:HD13	1.99	0.43
1:B:562:ASN:HD22	1:B:562:ASN:N	2.17	0.43
1:F:210:VAL:HG13	1:F:211:ASP:N	2.34	0.43
1:F:339:PHE:CE1	1:F:373:GLN:HB3	2.54	0.43
1:F:48:VAL:H	1:F:50:ASN:ND2	2.17	0.43
1:A:181:VAL:HG22	1:A:251:VAL:CG2	2.49	0.43
1:A:470:ASP:HB3	1:A:481:ILE:CD1	2.47	0.43
1:C:85:MET:CE	1:C:134:LYS:HG2	2.48	0.43
1:D:150:PRO:HG2	1:D:153:ASN:HA	2.01	0.43
1:E:37:VAL:HG21	1:E:441:LEU:HD22	2.00	0.43
1:E:505:VAL:HG23	1:E:578:VAL:HG22	1.99	0.43
1:F:268:ASN:HB2	1:F:287:LEU:HD12	2.01	0.43
1:F:266:PRO:HB2	1:F:288:SER:CB	2.49	0.43
1:A:265:VAL:HA	1:A:266:PRO:HD3	1.87	0.43
1:A:392:LEU:HB2	1:A:419:ILE:HD13	2.01	0.43
1:B:495:ALA:HB3	6:B:2264:HOH:O	2.18	0.43
1:C:248:VAL:HA	1:C:249:PRO:HD3	1.88	0.43
1:C:359:ASP:C	1:C:360:ARG:HG3	2.39	0.43
1:D:286:LYS:O	1:D:323:PRO:HD2	2.18	0.43
1:C:43:LEU:O	1:D:411:PRO:HB3	2.19	0.43
1:E:180:GLN:NE2	6:E:2081:HOH:O	2.48	0.43
1:E:282:ILE:HD12	1:E:328:PHE:CE2	2.54	0.43
1:B:295:ALA:HB2	1:B:314:VAL:HG21	2.00	0.43
1:C:152:PRO:HG2	1:C:154:ASP:OD2	2.18	0.43
1:D:339:PHE:CE1	1:D:373:GLN:HB3	2.54	0.43
1:E:315:ALA:HA	1:E:356:TYR:CG	2.54	0.43
1:E:494:VAL:HG13	1:E:518:LEU:HB2	2.00	0.43
1:E:521:VAL:HB	1:E:524:VAL:HG21	2.01	0.43
1:B:370:VAL:HG11	1:B:374:PRO:HG3	2.00	0.42
1:D:433:TYR:CG	1:D:434:ALA:N	2.87	0.42
1:D:470:ASP:HB3	1:D:481:ILE:CD1	2.49	0.42
1:E:531:VAL:HG11	1:F:125:GLN:CG	2.48	0.42
1:F:286:LYS:N	1:F:323:PRO:HG2	2.32	0.42
1:F:457:ASP:HA	1:F:458:PRO:HD3	1.81	0.42
1:F:504:LYS:HG2	1:F:577:LEU:HB2	2.01	0.42
1:F:538:GLU:C	1:F:539:ILE:HG13	2.40	0.42
1:F:75:ASN:ND2	1:F:102:ASN:HD21	2.17	0.42
1:B:117:LYS:HB2	1:B:175:MET:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:MET:HB2	1:D:515:ILE:HD13	2.01	0.42
1:E:558:TRP:CE2	1:F:147:PHE:HB3	2.54	0.42
1:C:478:ASN:ND2	1:C:492:THR:HG22	2.33	0.42
1:A:277:ASP:OD1	1:A:279:LYS:HG2	2.18	0.42
1:A:540:SER:HB3	1:A:541:PRO:CD	2.49	0.42
1:C:200:THR:HG22	1:C:225:VAL:HG22	2.01	0.42
1:C:376:HIS:HB2	1:C:437:HIS:O	2.20	0.42
1:C:67:LEU:HD23	1:C:118:ILE:HD12	2.00	0.42
1:E:56:GLY:O	1:E:60:THR:HG23	2.19	0.42
1:A:35:LEU:HD22	1:A:42:GLU:HA	2.01	0.42
1:C:456:ASN:H	1:C:456:ASN:ND2	2.16	0.42
1:D:275:SER:HA	1:D:276:PRO:HD3	1.92	0.42
1:D:453:TYR:CD1	1:D:543:GLN:HB2	2.55	0.42
1:F:548:THR:HG22	6:F:2026:HOH:O	2.19	0.42
1:B:50:ASN:N	1:B:50:ASN:HD22	2.00	0.42
1:B:452:ILE:CD1	1:B:542:GLN:HG3	2.49	0.42
1:D:540:SER:HB3	1:D:541:PRO:HD2	2.02	0.42
1:F:295:ALA:HB2	1:F:314:VAL:CG2	2.49	0.42
1:F:495:ALA:CA	6:F:2182:HOH:O	2.67	0.42
1:A:537:MET:CE	1:A:547:VAL:HG12	2.49	0.42
1:B:141:VAL:HB	1:B:170:ILE:HB	2.02	0.42
1:C:282:ILE:HD12	1:C:328:PHE:CE2	2.55	0.42
1:D:316:GLU:N	1:D:317:PRO:CD	2.83	0.42
1:F:363:TYR:CE1	1:F:364:ILE:HG13	2.54	0.42
1:B:370:VAL:HG13	1:B:415:GLN:HE21	1.85	0.42
1:C:269:PRO:HA	1:C:284:ASN:O	2.19	0.42
1:C:282:ILE:HG23	1:C:291:VAL:CG1	2.50	0.42
1:C:553:LYS:HB2	1:C:554:PRO:HD2	2.01	0.42
1:D:125:GLN:HG3	1:D:149:ILE:HD13	2.01	0.42
1:D:87:ASP:N	1:D:136:PRO:O	2.51	0.42
1:C:113:MET:HG3	1:D:406:VAL:O	2.20	0.42
1:D:456:ASN:HD22	1:D:456:ASN:N	2.15	0.42
1:E:575:ARG:HD3	6:E:2223:HOH:O	2.19	0.42
1:E:75:ASN:N	1:E:75:ASN:HD22	2.17	0.42
1:F:200:THR:HG22	1:F:225:VAL:HG22	2.00	0.42
1:F:77:ASP:HB2	6:F:2040:HOH:O	2.19	0.42
1:A:18:ASP:HB3	1:A:37:VAL:O	2.20	0.42
1:A:47:PRO:HA	1:A:50:ASN:HD21	1.85	0.42
1:F:262:TYR:CD1	1:F:262:TYR:N	2.88	0.42
1:F:538:GLU:HG2	1:F:539:ILE:N	2.34	0.42
1:A:372:TYR:O	1:A:396:SER:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:THR:HG22	1:A:499:GLY:HA3	2.01	0.42
1:A:520:MET:HB2	6:A:2308:HOH:O	2.19	0.42
1:C:205:ASN:OD1	1:C:208:ARG:N	2.53	0.42
1:D:368:LEU:HD23	1:D:369:ASP:N	2.34	0.42
1:D:371:GLN:CG	1:D:402:ARG:HD2	2.48	0.42
1:B:344:VAL:HG21	1:B:394:VAL:CG2	2.50	0.41
1:B:342:SER:HA	1:B:374:PRO:HD3	2.02	0.41
1:C:137:LYS:HG3	1:C:139:ASN:ND2	2.35	0.41
1:D:381:LEU:HD21	1:D:446:GLN:HE22	1.85	0.41
1:E:566:HIS:ND1	1:E:567:ALA:N	2.68	0.41
1:F:263:ILE:O	1:F:265:VAL:HG23	2.19	0.41
1:A:28:HIS:HA	1:A:77:ASP:HA	2.02	0.41
1:D:137:LYS:HG3	1:D:139:ASN:ND2	2.36	0.41
1:B:288:SER:C	1:B:290:THR:H	2.23	0.41
1:C:451:LYS:HE2	1:D:410:HIS:CE1	2.54	0.41
1:E:512:THR:HG22	1:E:514:TYR:CE1	2.56	0.41
1:E:568:LEU:HD13	1:F:212:LEU:HD21	2.01	0.41
1:F:282:ILE:HD12	1:F:328:PHE:CE2	2.56	0.41
1:B:495:ALA:N	6:B:2265:HOH:O	2.53	0.41
1:B:49:PHE:CZ	1:B:99:ASP:HB2	2.56	0.41
1:C:365:ARG:HH11	1:C:365:ARG:HG3	1.85	0.41
1:C:372:TYR:HE2	1:C:402:ARG:HG2	1.84	0.41
1:C:568:LEU:HD21	1:D:287:LEU:HD21	2.00	0.41
1:E:494:VAL:HG22	6:E:2205:HOH:O	2.19	0.41
1:F:32:VAL:HG23	1:F:48:VAL:HG21	2.02	0.41
1:C:308:GLU:O	1:C:311:ASP:HB2	2.20	0.41
1:D:265:VAL:CG1	1:D:266:PRO:HD2	2.49	0.41
1:E:562:ASN:N	1:E:562:ASN:HD22	2.17	0.41
1:A:518:LEU:HD13	6:A:2282:HOH:O	2.20	0.41
1:B:371:GLN:CG	1:B:402:ARG:HD2	2.51	0.41
1:C:327:THR:HG22	1:C:377:ASN:ND2	2.35	0.41
1:D:57:TRP:CZ2	1:D:115:THR:HB	2.55	0.41
1:D:376:HIS:CE1	1:D:438:ASP:HB2	2.56	0.41
1:A:540:SER:HB3	1:A:541:PRO:HD2	2.02	0.41
1:A:78:CYS:HB2	1:A:97:ILE:HG12	2.02	0.41
1:A:538:GLU:OE2	1:B:409:LEU:HG	2.21	0.41
1:C:130:LEU:HA	1:C:142:PHE:O	2.21	0.41
1:C:363:TYR:CE1	1:C:364:ILE:HG13	2.55	0.41
1:D:127:ILE:HA	1:D:144:ASN:O	2.21	0.41
1:D:308:GLU:O	1:D:311:ASP:HB2	2.20	0.41
1:D:78:CYS:HB2	1:D:97:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:THR:O	1:A:175:MET:HB2	2.20	0.41
1:A:575:ARG:NH2	1:B:158:PHE:O	2.54	0.41
1:B:261:ARG:HA	6:B:2151:HOH:O	2.19	0.41
1:B:513:VAL:O	1:B:546:SER:HA	2.21	0.41
1:C:107:ARG:NH1	1:C:116:ASP:OD2	2.48	0.41
1:D:35:LEU:CD2	1:D:42:GLU:HA	2.51	0.41
1:D:492:THR:HG22	1:D:499:GLY:HA3	2.03	0.41
1:D:75:ASN:N	1:D:75:ASN:HD22	2.17	0.41
1:D:95:LEU:HD23	1:D:95:LEU:C	2.41	0.41
1:E:109:ARG:HB3	1:E:111:ASP:OD1	2.20	0.41
1:F:354:LYS:O	1:F:359:ASP:HB2	2.20	0.41
1:A:11:HIS:HB3	6:A:2001:HOH:O	2.21	0.41
1:B:117:LYS:CB	1:B:175:MET:HG3	2.51	0.41
1:B:386:ASP:O	1:B:387:ALA:C	2.59	0.41
1:B:470:ASP:HB3	1:B:481:ILE:CD1	2.43	0.41
1:C:95:LEU:HD22	1:C:108:ILE:HD12	2.03	0.41
1:D:180:GLN:HG3	1:D:248:VAL:HG11	2.02	0.41
1:D:266:PRO:HB2	1:D:288:SER:OG	2.20	0.41
1:D:37:VAL:CG1	1:D:38:PRO:HA	2.51	0.41
1:C:287:LEU:HD21	1:D:568:LEU:HD21	2.03	0.41
1:E:131:ARG:HD2	1:E:191:ASP:CG	2.41	0.41
1:E:371:GLN:HG2	1:E:402:ARG:HD2	2.02	0.41
1:E:61:ASN:ND2	1:E:548:THR:HG22	2.35	0.41
1:A:410:HIS:CE1	1:B:451:LYS:HE3	2.55	0.41
1:C:49:PHE:CZ	1:C:99:ASP:HB2	2.56	0.41
1:F:361:VAL:HG12	1:F:362:ASN:N	2.36	0.41
1:F:449:THR:HB	6:F:2150:HOH:O	2.20	0.41
1:C:366:GLN:HG2	1:C:367:LYS:N	2.36	0.41
1:C:435:GLU:HA	1:C:436:PRO:HD2	2.03	0.41
1:D:282:ILE:HD12	1:D:328:PHE:CE2	2.56	0.41
1:D:295:ALA:HB2	1:D:314:VAL:CG2	2.51	0.41
1:D:321:LEU:HB3	1:D:340:ILE:HD12	2.02	0.41
1:F:37:VAL:HG21	1:F:441:LEU:HD22	2.03	0.41
1:B:291:VAL:O	1:B:316:GLU:HA	2.21	0.40
1:C:57:TRP:CH2	1:C:115:THR:HB	2.56	0.40
1:C:207:GLU:HG3	1:C:218:ASN:ND2	2.36	0.40
1:C:433:TYR:CG	1:C:434:ALA:N	2.88	0.40
1:C:27:GLY:O	1:C:77:ASP:HA	2.21	0.40
1:D:109:ARG:HD2	1:D:111:ASP:OD1	2.20	0.40
1:D:155:GLY:HA2	1:D:158:PHE:CE1	2.56	0.40
1:F:268:ASN:O	1:F:286:LYS:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:325:HIS:CD2	1:F:376:HIS:HA	2.56	0.40
1:F:344:VAL:HG21	1:F:394:VAL:CG2	2.51	0.40
1:F:376:HIS:HB2	1:F:437:HIS:O	2.21	0.40
1:A:297:ASP:HB2	6:A:2178:HOH:O	2.20	0.40
1:B:365:ARG:HG3	1:B:365:ARG:HH11	1.86	0.40
1:B:478:ASN:HA	1:B:490:TYR:O	2.21	0.40
1:D:135:VAL:HG13	1:D:136:PRO:HA	2.03	0.40
1:E:151:GLN:HA	1:E:152:PRO:HA	2.00	0.40
1:F:343:GLN:HE22	1:F:367:LYS:HD3	1.82	0.40
1:F:494:VAL:HG22	6:F:2186:HOH:O	2.22	0.40
1:F:78:CYS:HA	1:F:98:ASN:O	2.21	0.40
1:A:212:LEU:HD21	1:B:568:LEU:HD13	2.03	0.40
1:A:514:TYR:CD2	1:A:546:SER:HB3	2.56	0.40
1:B:174:THR:CG2	1:B:176:ASP:OD2	2.69	0.40
1:B:344:VAL:HG21	1:B:394:VAL:HG21	2.03	0.40
1:C:147:PHE:HB3	1:D:558:TRP:CE2	2.56	0.40
1:C:131:ARG:HD2	1:C:191:ASP:CG	2.42	0.40
1:C:363:TYR:CD1	1:C:364:ILE:HG13	2.57	0.40
1:C:412:GLU:HG3	1:C:436:PRO:HD2	2.02	0.40
1:D:130:LEU:C	1:D:130:LEU:HD23	2.42	0.40
1:E:67:LEU:HD23	1:E:118:ILE:CD1	2.51	0.40
1:F:39:SER:O	1:F:40:MET:HB2	2.22	0.40
1:C:316:GLU:N	1:C:317:PRO:CD	2.84	0.40
1:E:100:LYS:HG3	1:E:126:ALA:HB1	2.04	0.40
1:F:288:SER:C	1:F:290:THR:H	2.24	0.40
1:F:314:VAL:HG12	1:F:314:VAL:O	2.21	0.40
1:A:189:ASN:O	1:A:201:SER:HA	2.21	0.40
1:A:200:THR:HG21	1:A:225:VAL:HG22	2.01	0.40
1:B:308:GLU:O	1:B:311:ASP:HB2	2.21	0.40
1:C:342:SER:HA	1:C:374:PRO:CD	2.49	0.40
1:E:328:PHE:CD1	1:E:328:PHE:N	2.89	0.40
1:F:533:HIS:O	1:F:535:VAL:HG23	2.21	0.40
1:F:548:THR:HG21	6:F:2025:HOH:O	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	570/581 (98%)	532 (93%)	31 (5%)	7 (1%)	13	19
1	B	570/581 (98%)	527 (92%)	35 (6%)	8 (1%)	11	15
1	C	570/581 (98%)	521 (91%)	41 (7%)	8 (1%)	11	15
1	D	570/581 (98%)	517 (91%)	44 (8%)	9 (2%)	9	13
1	E	570/581 (98%)	519 (91%)	47 (8%)	4 (1%)	22	32
1	F	570/581 (98%)	519 (91%)	45 (8%)	6 (1%)	14	20
All	All	3420/3486 (98%)	3135 (92%)	243 (7%)	42 (1%)	13	19

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	LYS
1	A	495	ALA
1	B	267	LYS
1	C	267	LYS
1	D	267	LYS
1	D	495	ALA
1	E	267	LYS
1	F	267	LYS
1	F	495	ALA
1	B	495	ALA
1	C	286	LYS
1	C	495	ALA
1	E	286	LYS
1	E	495	ALA
1	F	359	ASP
1	A	286	LYS
1	A	434	ALA
1	B	286	LYS
1	D	434	ALA
1	A	435	GLU

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Mol	Chain	Res	Type
1	B	217	ARG
1	B	400	LYS
1	B	434	ALA
1	C	434	ALA
1	D	400	LYS
1	F	434	ALA
1	F	435	GLU
1	B	435	GLU
1	C	435	GLU
1	D	286	LYS
1	D	435	GLU
1	E	435	GLU
1	A	359	ASP
1	C	217	ARG
1	D	373	GLN
1	F	286	LYS
1	C	289	PRO
1	D	496	PRO
1	C	373	GLN
1	A	289	PRO
1	B	373	GLN
1	D	289	PRO

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	491/497 (99%)	474 (96%)	17 (4%)	36	55
1	B	491/497 (99%)	469 (96%)	22 (4%)	27	44
1	C	491/497 (99%)	474 (96%)	17 (4%)	36	55
1	D	491/497 (99%)	476 (97%)	15 (3%)	40	60
1	E	491/497 (99%)	473 (96%)	18 (4%)	34	53
1	F	491/497 (99%)	471 (96%)	20 (4%)	30	48
All	All	2946/2982 (99%)	2837 (96%)	109 (4%)	34	53

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	75	ASN
1	A	124	VAL
1	A	161	ASP
1	A	186	ASN
1	A	212	LEU
1	A	304	GLU
1	A	328	PHE
1	A	359	ASP
1	A	368	LEU
1	A	409	LEU
1	A	451	LYS
1	A	456	ASN
1	A	548	THR
1	A	562	ASN
1	A	563	TRP
1	A	564	PHE
1	B	50	ASN
1	B	70	ASP
1	B	75	ASN
1	B	98	ASN
1	B	103	THR
1	B	124	VAL
1	B	186	ASN
1	B	212	LEU
1	B	261	ARG
1	B	304	GLU
1	B	328	PHE
1	B	359	ASP
1	B	368	LEU
1	B	390	LYS
1	B	409	LEU
1	B	452	ILE
1	B	456	ASN
1	B	492	THR
1	B	548	THR
1	B	562	ASN
1	B	563	TRP
1	B	564	PHE
1	C	50	ASN
1	C	75	ASN
1	C	124	VAL

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Mol	Chain	Res	Type
1	C	186	ASN
1	C	212	LEU
1	C	273	ASN
1	C	359	ASP
1	C	360	ARG
1	C	390	LYS
1	C	409	LEU
1	C	451	LYS
1	C	456	ASN
1	C	520	MET
1	C	548	THR
1	C	562	ASN
1	C	563	TRP
1	C	564	PHE
1	D	24	TRP
1	D	50	ASN
1	D	75	ASN
1	D	98	ASN
1	D	124	VAL
1	D	186	ASN
1	D	212	LEU
1	D	359	ASP
1	D	409	LEU
1	D	451	LYS
1	D	456	ASN
1	D	548	THR
1	D	562	ASN
1	D	563	TRP
1	D	564	PHE
1	E	50	ASN
1	E	75	ASN
1	E	124	VAL
1	E	186	ASN
1	E	212	LEU
1	E	261	ARG
1	E	359	ASP
1	E	368	LEU
1	E	390	LYS
1	E	409	LEU
1	E	451	LYS
1	E	456	ASN
1	E	540	SER

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Mol	Chain	Res	Type
1	E	548	THR
1	E	561	CYS
1	E	562	ASN
1	E	563	TRP
1	E	564	PHE
1	F	24	TRP
1	F	50	ASN
1	F	70	ASP
1	F	75	ASN
1	F	78	CYS
1	F	103	THR
1	F	124	VAL
1	F	161	ASP
1	F	186	ASN
1	F	212	LEU
1	F	261	ARG
1	F	359	ASP
1	F	409	LEU
1	F	452	ILE
1	F	456	ASN
1	F	492	THR
1	F	548	THR
1	F	562	ASN
1	F	563	TRP
1	F	564	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	71	GLN
1	A	72	GLN
1	A	75	ASN
1	A	98	ASN
1	A	125	GLN
1	A	139	ASN
1	A	144	ASN
1	A	151	GLN
1	A	180	GLN
1	A	186	ASN
1	A	189	ASN
1	A	218	ASN

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Mol	Chain	Res	Type
1	A	343	GLN
1	A	362	ASN
1	A	366	GLN
1	A	371	GLN
1	A	373	GLN
1	A	410	HIS
1	A	415	GLN
1	A	446	GLN
1	A	456	ASN
1	A	517	ASN
1	A	543	GLN
1	A	562	ASN
1	B	50	ASN
1	B	61	ASN
1	B	71	GLN
1	B	75	ASN
1	B	98	ASN
1	B	125	GLN
1	B	139	ASN
1	B	144	ASN
1	B	151	GLN
1	B	186	ASN
1	B	189	ASN
1	B	284	ASN
1	B	343	GLN
1	B	362	ASN
1	B	366	GLN
1	B	371	GLN
1	B	373	GLN
1	B	410	HIS
1	B	415	GLN
1	B	446	GLN
1	B	456	ASN
1	B	543	GLN
1	B	562	ASN
1	C	50	ASN
1	C	61	ASN
1	C	71	GLN
1	C	72	GLN
1	C	75	ASN
1	C	98	ASN
1	C	125	GLN

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Mol	Chain	Res	Type
1	C	139	ASN
1	C	151	GLN
1	C	186	ASN
1	C	284	ASN
1	C	343	GLN
1	C	362	ASN
1	C	366	GLN
1	C	371	GLN
1	C	413	ASN
1	C	415	GLN
1	C	446	GLN
1	C	456	ASN
1	C	543	GLN
1	C	562	ASN
1	D	50	ASN
1	D	61	ASN
1	D	71	GLN
1	D	72	GLN
1	D	75	ASN
1	D	98	ASN
1	D	120	HIS
1	D	125	GLN
1	D	139	ASN
1	D	151	GLN
1	D	180	GLN
1	D	186	ASN
1	D	218	ASN
1	D	343	GLN
1	D	362	ASN
1	D	366	GLN
1	D	371	GLN
1	D	413	ASN
1	D	415	GLN
1	D	446	GLN
1	D	456	ASN
1	D	543	GLN
1	D	562	ASN
1	E	50	ASN
1	E	61	ASN
1	E	71	GLN
1	E	72	GLN
1	E	75	ASN

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Mol	Chain	Res	Type
1	E	98	ASN
1	E	125	GLN
1	E	139	ASN
1	E	144	ASN
1	E	151	GLN
1	E	180	GLN
1	E	186	ASN
1	E	189	ASN
1	E	284	ASN
1	E	343	GLN
1	E	362	ASN
1	E	366	GLN
1	E	371	GLN
1	E	373	GLN
1	E	410	HIS
1	E	415	GLN
1	E	446	GLN
1	E	456	ASN
1	E	478	ASN
1	E	543	GLN
1	E	562	ASN
1	F	50	ASN
1	F	61	ASN
1	F	71	GLN
1	F	72	GLN
1	F	75	ASN
1	F	98	ASN
1	F	125	GLN
1	F	139	ASN
1	F	144	ASN
1	F	151	GLN
1	F	186	ASN
1	F	189	ASN
1	F	284	ASN
1	F	343	GLN
1	F	362	ASN
1	F	366	GLN
1	F	377	ASN
1	F	410	HIS
1	F	415	GLN
1	F	446	GLN
1	F	456	ASN

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Mol	Chain	Res	Type
1	F	543	GLN
1	F	562	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 18 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CUA	F	701	1	0,1,1	0.00	-	-		
2	CUA	D	701	1	0,1,1	0.00	-	-		
3	CUZ	A	801	1,6	0,9,9	0.00	-	-		
2	CUA	A	701	-	0,1,1	0.00	-	-		
2	CUA	E	701	1	0,1,1	0.00	-	-		
3	CUZ	D	801	1,6	0,9,9	0.00	-	-		
3	CUZ	E	801	1,6	0,9,9	0.00	-	-		
3	CUZ	F	801	1,6	0,9,9	0.00	-	-		
3	CUZ	C	801	1,6	0,9,9	0.00	-	-		
2	CUA	C	701	1	0,1,1	0.00	-	-		
3	CUZ	B	801	1,6	0,9,9	0.00	-	-		
2	CUA	B	701	-	0,1,1	0.00	-	-		

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	801	CUZ	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	572/581 (98%)	-0.08	17 (2%)	50 49	31, 52, 71, 91	3 (0%)
1	B	572/581 (98%)	-0.04	24 (4%)	36 35	32, 52, 71, 91	3 (0%)
1	C	572/581 (98%)	0.25	41 (7%)	15 14	41, 60, 77, 91	3 (0%)
1	D	572/581 (98%)	0.06	20 (3%)	44 43	39, 58, 76, 92	3 (0%)
1	E	572/581 (98%)	0.02	21 (3%)	41 41	35, 54, 71, 89	3 (0%)
1	F	572/581 (98%)	0.19	23 (4%)	38 37	34, 58, 75, 91	3 (0%)
All	All	3432/3486 (98%)	0.07	146 (4%)	35 33	31, 56, 74, 92	18 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	314	VAL	5.0
1	C	360	ARG	4.9
1	C	362	ASN	4.7
1	A	201	SER	4.6
1	F	361	VAL	4.4
1	B	360	ARG	4.4
1	F	360	ARG	4.4
1	C	354	LYS	4.2
1	B	272	LEU	4.0
1	F	307	ILE	4.0
1	A	360	ARG	3.9
1	D	361	VAL	3.9
1	B	190	THR	3.8
1	D	581	ALA	3.8
1	A	272	LEU	3.6
1	B	201	SER	3.5
1	E	581	ALA	3.5
1	C	87	ASP	3.5
1	C	361	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	471	GLY	3.4
1	F	164	TYR	3.4
1	A	187	LEU	3.4
1	C	256	GLU	3.3
1	A	199	ALA	3.3
1	C	423	GLU	3.3
1	A	202	THR	3.3
1	C	425	LYS	3.3
1	C	358	GLY	3.2
1	F	581	ALA	3.2
1	D	345	CYS	3.2
1	F	256	GLU	3.2
1	D	573	VAL	3.1
1	F	362	ASN	3.1
1	D	358	GLY	3.1
1	C	581	ALA	3.1
1	B	273	ASN	3.0
1	A	224	VAL	3.0
1	D	256	GLU	3.0
1	D	360	ARG	3.0
1	B	271	GLY	3.0
1	C	86	THR	2.9
1	B	129	GLY	2.9
1	E	199	ALA	2.9
1	C	427	VAL	2.9
1	C	10	ALA	2.9
1	E	200	THR	2.9
1	D	427	VAL	2.8
1	A	144	ASN	2.8
1	C	239	ASN	2.8
1	A	126	ALA	2.8
1	A	190	THR	2.8
1	E	272	LEU	2.8
1	F	255	GLY	2.8
1	F	216	MET	2.8
1	C	363	TYR	2.8
1	A	200	THR	2.8
1	C	309	LEU	2.8
1	C	365	ARG	2.7
1	A	81	PRO	2.7
1	B	192	ALA	2.7
1	C	307	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	280	TYR	2.7
1	C	308	GLU	2.7
1	B	191	ASP	2.7
1	B	282	ILE	2.7
1	C	237	ALA	2.7
1	D	11	HIS	2.7
1	C	350	ALA	2.7
1	B	202	THR	2.6
1	B	281	PHE	2.6
1	D	362	ASN	2.6
1	E	474	LEU	2.6
1	B	189	ASN	2.6
1	C	88	GLY	2.6
1	C	241	LYS	2.6
1	C	355	HIS	2.6
1	C	357	ASN	2.6
1	C	302	LEU	2.6
1	F	184	ASP	2.6
1	D	306	LYS	2.5
1	B	361	VAL	2.5
1	F	156	THR	2.5
1	D	363	TYR	2.5
1	F	573	VAL	2.5
1	C	419	ILE	2.5
1	B	274	THR	2.5
1	B	143	CYS	2.4
1	D	241	LYS	2.4
1	B	326	THR	2.4
1	F	237	ALA	2.4
1	E	577	LEU	2.4
1	D	161	ASP	2.4
1	C	238	GLY	2.4
1	C	424	MET	2.4
1	D	190	THR	2.4
1	F	264	PRO	2.4
1	E	130	LEU	2.4
1	C	417	ILE	2.4
1	B	199	ALA	2.4
1	B	283	ALA	2.4
1	E	201	SER	2.4
1	F	206	SER	2.4
1	A	129	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	566	HIS	2.3
1	E	190	THR	2.3
1	E	496	PRO	2.3
1	C	85	MET	2.3
1	B	573	VAL	2.3
1	E	485	ASN	2.3
1	F	357	ASN	2.3
1	B	200	THR	2.3
1	D	200	THR	2.3
1	C	242	THR	2.3
1	F	219	ASP	2.3
1	A	130	LEU	2.3
1	A	529	CYS	2.3
1	B	11	HIS	2.2
1	E	143	CYS	2.2
1	E	573	VAL	2.2
1	C	359	ASP	2.2
1	E	578	VAL	2.2
1	A	282	ILE	2.2
1	F	303	PHE	2.2
1	B	224	VAL	2.2
1	F	200	THR	2.2
1	E	554	PRO	2.2
1	F	212	LEU	2.2
1	E	503	PHE	2.1
1	C	299	LEU	2.1
1	C	311	ASP	2.1
1	C	315	ALA	2.1
1	B	131	ARG	2.1
1	E	470	ASP	2.1
1	D	143	CYS	2.1
1	C	173	GLU	2.1
1	F	233	ALA	2.1
1	C	136	PRO	2.1
1	C	471	GLY	2.1
1	F	157	ASP	2.1
1	A	189	ASN	2.1
1	E	360	ARG	2.1
1	C	11	HIS	2.0
1	D	354	LYS	2.0
1	E	11	HIS	2.0
1	F	306	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	10	ALA	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 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CUZ	C	801	5/5	0.92	0.09	62,65,66,67	0
3	CUZ	D	801	5/5	0.93	0.08	59,61,62,64	0
5	CL	D	902	1/1	0.94	0.21	71,71,71,71	0
3	CUZ	F	801	5/5	0.94	0.08	61,61,63,63	0
4	CA	F	901	1/1	0.94	0.05	67,67,67,67	0
4	CA	D	903	1/1	0.95	0.12	70,70,70,70	0
4	CA	F	903	1/1	0.95	0.08	67,67,67,67	0
4	CA	C	903	1/1	0.95	0.08	63,63,63,63	0
4	CA	D	901	1/1	0.96	0.06	64,64,64,64	0
3	CUZ	E	801	5/5	0.96	0.12	44,45,47,48	0
4	CA	A	901	1/1	0.97	0.08	46,46,46,46	0
5	CL	F	902	1/1	0.97	0.30	73,73,73,73	0
3	CUZ	A	801	5/5	0.97	0.11	43,44,45,48	0
3	CUZ	B	801	5/5	0.97	0.10	44,44,47,50	0
2	CUA	F	701	2/2	0.98	0.07	38,38,38,38	0
4	CA	B	901	1/1	0.98	0.08	50,50,50,50	0
2	CUA	D	701	2/2	0.98	0.05	54,54,54,57	0
2	CUA	C	701	2/2	0.98	0.05	57,57,57,58	0
5	CL	C	902	1/1	0.98	0.25	75,75,75,75	0
2	CUA	A	701	2/2	0.98	0.07	47,47,47,47	0
4	CA	C	901	1/1	0.98	0.04	63,63,63,63	0
2	CUA	E	701	2/2	0.98	0.06	56,56,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CA	B	903	1/1	0.98	0.07	49,49,49,49	0
5	CL	A	902	1/1	0.99	0.16	44,44,44,44	0
4	CA	E	901	1/1	0.99	0.07	41,41,41,41	0
4	CA	A	903	1/1	0.99	0.08	41,41,41,41	0
5	CL	E	902	1/1	0.99	0.14	46,46,46,46	0
4	CA	E	903	1/1	0.99	0.08	47,47,47,47	0
5	CL	B	902	1/1	0.99	0.14	43,43,43,43	0
2	CUA	B	701	2/2	0.99	0.07	37,37,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.