



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:01 PM UTC

PDB ID : 1MTY / pdb_00001mty
Title : METHANE MONOOXYGENASE HYDROXYLASE FROM METHYLOCOCCUS CAPSULATUS (BATH)
Authors : Rosenzweig, A.C.; Nordlund, P.; Lippard, S.J.; Frederick, C.A.
Deposited on : 1996-07-10
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

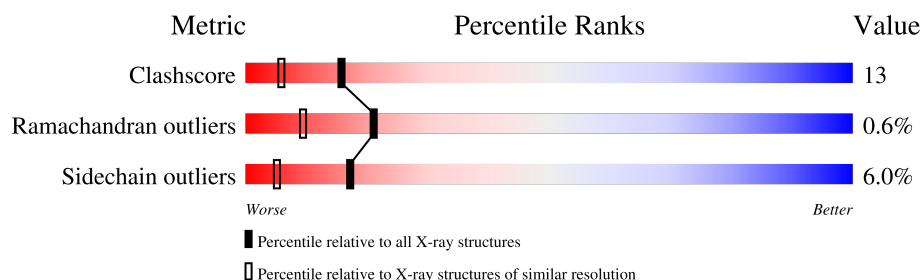
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	512	
1	E	512	
2	B	384	
2	C	384	
3	G	162	
3	H	162	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25065 atoms, of which 6193 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 METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	512	Total	C	H	N	O	S	0	0	0
			5120	2680	934	721	767	18			
1	E	512	Total	C	H	N	O	S	0	0	0
			5120	2680	934	721	767	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	306	ASP	ASN	conflict	UNP P22869
D	444	GLU	GLN	conflict	UNP P22869
E	306	ASP	ASN	conflict	UNP P22869
E	444	GLU	GLN	conflict	UNP P22869

- Molecule 2 is a protein called METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	384	Total	C	N	O	S		0	0	0
			3167	2038	547	575	7				
2	C	384	Total	C	H	N	O	S	0	0	0
			3874	2038	707	547	575	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	142	ASP	THR	conflict	UNP P18798
B	143	GLU	SER	conflict	UNP P18798
B	144	PHE	SER	conflict	UNP P18798
B	145	ILE	CYS	conflict	UNP P18798
C	142	ASP	THR	conflict	UNP P18798
C	143	GLU	SER	conflict	UNP P18798
C	144	PHE	SER	conflict	UNP P18798
C	145	ILE	CYS	conflict	UNP P18798

- Molecule 3 is a protein called METHANE MONOOXYGENASE HYDROXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			
3	H	162	Total	C	H	N	O	S	0	0	0
			1658	847	321	241	244	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	38	ASP	HIS	conflict	UNP P11987
G	80	LYS	ASN	conflict	UNP P11987
H	38	ASP	HIS	conflict	UNP P11987
H	80	LYS	ASN	conflict	UNP P11987

- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Fe	0	0
			2	2		
4	E	2	Total	Fe	0	0
			2	2		

- Molecule 5 is water.

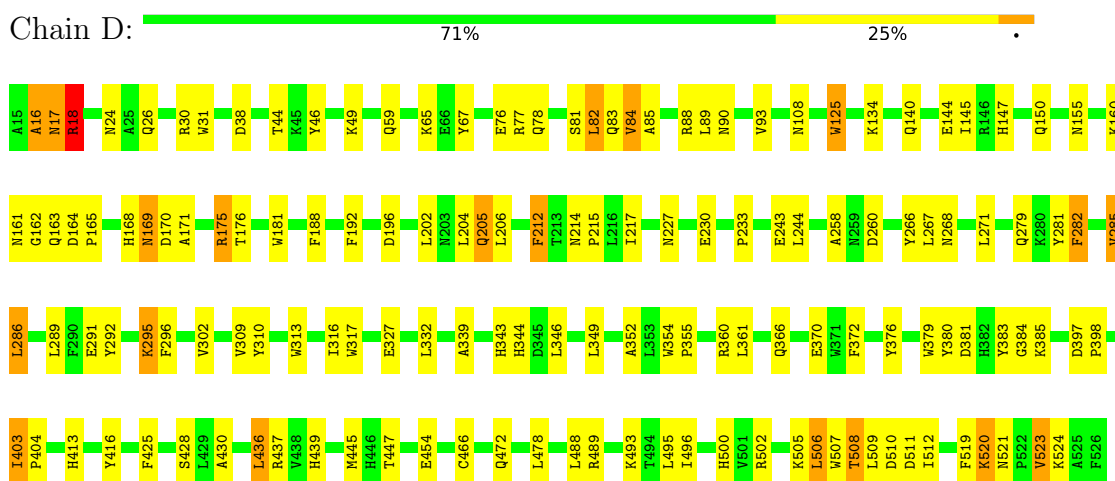
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	292	Total	H	O	0	0
			876	584	292		
5	E	308	Total	H	O	0	0
			924	616	308		
5	B	263	Total	H	O	0	0
			789	526	263		
5	C	269	Total	H	O	0	0
			807	538	269		
5	G	157	Total	H	O	0	0
			471	314	157		
5	H	199	Total	H	O	0	0
			597	398	199		

3 Residue-property plots

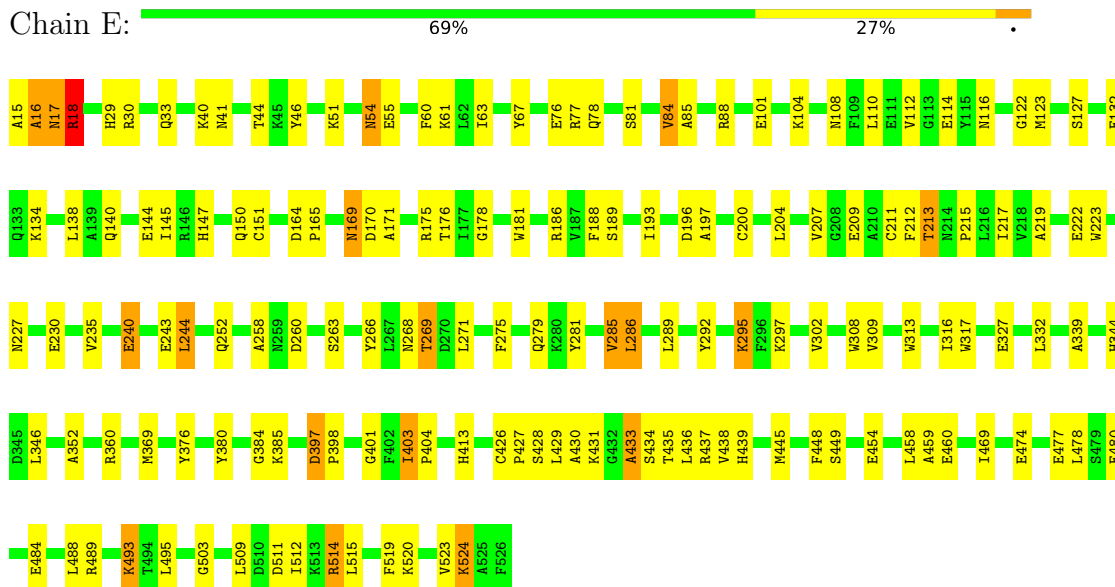
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: METHANE MONOOXYGENASE HYDROXYLASE

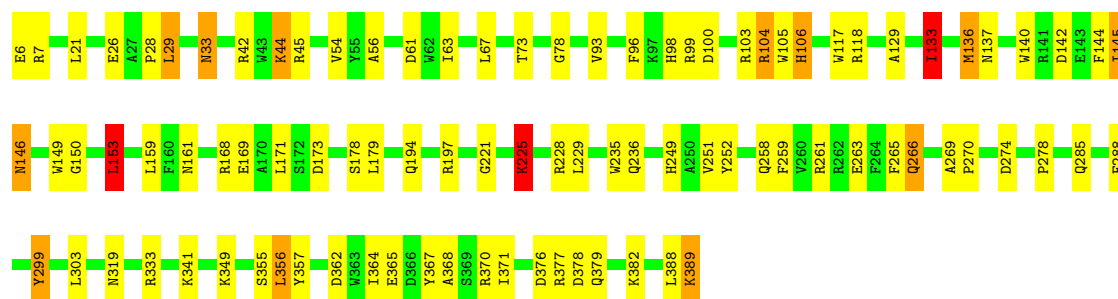


• Molecule 1: METHANE MONOOXYGENASE HYDROXYLASE



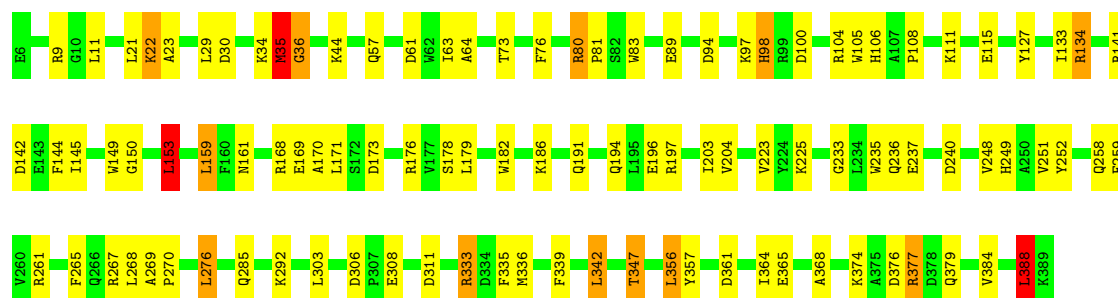
• Molecule 2: METHANE MONOOXYGENASE HYDROXYLASE

Chain B:  76% 21% . .



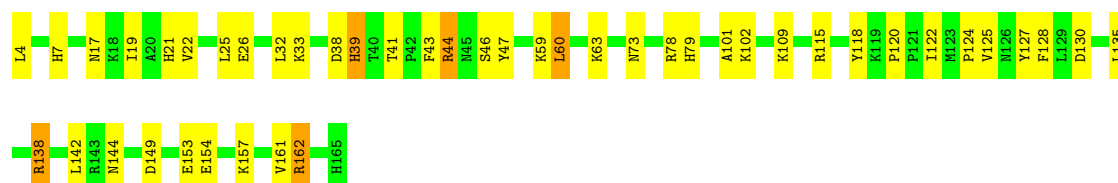
• Molecule 2: METHANE MONOOXYGENASE HYDROXYLASE

Chain C:  73% 23% . .



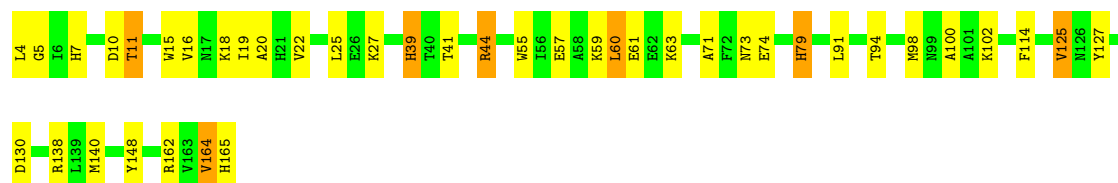
• Molecule 3: METHANE MONOOXYGENASE HYDROXYLASE

Chain G:  72% 25% .



• Molecule 3: METHANE MONOOXYGENASE HYDROXYLASE

Chain H:  75% 21% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.70Å 109.60Å 330.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 1.70	Depositor
% Data completeness (in resolution range)	77.0 (5.00-1.70)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25065	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	D	0.57	0/4311	1.02	26/5855 (0.4%)
1	E	0.59	0/4311	1.05	27/5855 (0.5%)
2	B	0.60	1/3263 (0.0%)	0.98	24/4430 (0.5%)
2	C	0.57	0/3263	0.97	19/4430 (0.4%)
3	G	0.58	0/1366	0.96	8/1840 (0.4%)
3	H	0.60	0/1366	0.99	8/1840 (0.4%)
All	All	0.58	1/17880 (0.0%)	1.01	112/24250 (0.5%)

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
2	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	136	MET	SD-CE	-5.50	1.65	1.79

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	339	ALA	N-CA-C	9.27	121.15	111.14
1	E	316	ILE	N-CA-C	9.20	119.23	110.30
1	E	339	ALA	N-CA-C	9.15	120.95	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	ASN	N-CA-C	-9.04	99.29	110.41
2	B	133	ILE	CB-CA-C	-8.32	99.27	112.16
2	C	105	TRP	N-CA-C	-7.68	98.89	109.95
2	C	144	PHE	N-CA-C	7.64	119.39	111.14
1	D	295	LYS	N-CA-C	-7.62	101.22	111.96
2	C	236	GLN	N-CA-C	7.45	122.37	113.28
1	D	258	ALA	N-CA-C	7.25	120.23	111.82
3	H	5	GLY	N-CA-C	7.25	124.48	112.30
2	B	104	ARG	N-CA-C	7.25	120.54	108.73
1	E	426	CYS	CA-C-N	7.23	127.56	119.32
1	E	426	CYS	C-N-CA	7.23	127.56	119.32
1	D	243	GLU	N-CA-C	7.14	119.07	111.28
1	D	16	ALA	N-CA-C	7.12	121.06	110.52
1	D	430	ALA	N-CA-C	7.12	120.28	110.24
1	E	266	TYR	N-CA-C	6.99	122.71	114.04
1	E	295	LYS	N-CA-C	-6.88	102.26	111.96
2	B	103	ARG	CA-C-N	-6.74	113.80	122.77
2	B	103	ARG	C-N-CA	-6.74	113.80	122.77
1	E	433	ALA	N-CA-C	6.65	124.97	110.80
1	E	478	LEU	N-CA-C	6.59	119.02	111.11
2	B	63	ILE	N-CA-C	-6.57	96.84	107.28
3	H	79	HIS	N-CA-C	6.57	122.26	113.72
1	E	258	ALA	N-CA-C	6.56	119.25	111.71
1	D	266	TYR	N-CA-C	6.51	122.71	114.31
1	D	285	VAL	N-CA-C	6.51	116.67	110.42
3	G	130	ASP	N-CA-C	-6.51	104.27	111.36
2	B	144	PHE	N-CA-C	6.47	118.13	111.14
2	B	146	ASN	N-CA-C	6.41	117.93	111.07
1	D	205	GLN	N-CA-C	6.39	119.49	111.24
1	D	93	VAL	N-CA-C	6.38	117.30	111.81
2	C	252	TYR	N-CA-C	6.38	117.92	110.97
1	D	309	VAL	N-CA-C	6.36	116.99	110.82
2	B	54	VAL	N-CA-C	6.32	117.46	108.93
1	E	85	ALA	N-CA-C	6.29	118.66	111.11
1	E	403	ILE	N-CA-C	-6.29	100.13	107.61
1	E	122	GLY	N-CA-C	-6.27	104.74	112.77
1	D	316	ILE	N-CA-C	6.24	116.29	110.42
3	G	73	ASN	N-CA-C	-6.23	102.49	110.53
1	D	380	TYR	N-CA-C	6.20	117.70	111.07
2	C	169	GLU	N-CA-C	6.15	120.95	113.38
1	E	285	VAL	N-CA-C	6.12	116.29	110.42
1	E	145	ILE	N-CA-C	-6.08	104.58	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	162	ARG	N-CA-C	-5.99	97.97	108.20
3	H	130	ASP	N-CA-C	-5.98	104.89	111.82
1	D	282	PHE	N-CA-C	5.94	118.71	111.82
3	G	118	TYR	N-CA-C	5.93	121.24	113.30
1	E	430	ALA	N-CA-C	5.87	118.57	110.35
1	D	267	LEU	N-CA-C	5.87	118.16	111.11
2	B	169	GLU	N-CA-C	5.86	120.59	113.38
2	C	106	HIS	N-CA-C	5.85	118.13	111.11
2	C	142	ASP	N-CA-C	5.84	117.73	111.36
1	D	145	ILE	N-CA-C	-5.84	104.82	110.72
2	C	98	HIS	N-CA-C	5.80	118.42	110.24
1	E	243	GLU	N-CA-C	5.76	118.33	111.71
1	E	397	ASP	N-CA-C	5.75	117.78	109.04
1	E	431	LYS	N-CA-C	-5.74	106.27	113.28
2	B	236	GLN	N-CA-C	5.74	120.56	113.50
2	B	265	PHE	N-CA-C	5.71	117.31	111.14
2	B	149	TRP	N-CA-C	-5.69	105.16	111.36
1	D	212	PHE	N-CA-C	5.68	119.92	112.13
2	B	142	ASP	N-CA-C	5.65	118.37	111.82
2	C	388	LEU	N-CA-C	5.63	122.80	110.80
2	B	225	LYS	N-CA-C	5.57	117.82	111.02
2	B	106	HIS	N-CA-C	5.55	117.01	111.07
2	C	249	HIS	N-CA-C	5.54	119.22	112.23
1	D	291	GLU	N-CA-C	5.53	117.39	111.36
3	G	149	ASP	N-CA-C	5.47	117.33	111.36
2	B	249	HIS	N-CA-C	5.47	119.12	112.23
2	B	299	TYR	N-CA-C	5.45	118.14	111.82
3	H	71	ALA	N-CA-C	5.44	117.01	111.14
2	C	63	ILE	N-CA-C	-5.43	98.64	107.28
2	B	56	ALA	N-CA-C	-5.41	105.55	111.82
2	C	306	ASP	CA-C-N	5.40	125.74	119.47
2	C	306	ASP	C-N-CA	5.40	125.74	119.47
1	D	162	GLY	N-CA-C	5.39	120.85	112.60
1	D	17	ASN	N-CA-C	-5.39	99.32	110.80
2	C	153	LEU	CA-CB-CG	5.37	135.08	116.30
1	D	496	ILE	N-CA-C	-5.36	105.49	110.53
1	D	85	ALA	N-CA-C	5.31	117.49	111.11
1	D	164	ASP	CA-C-N	5.30	124.81	119.19
1	D	164	ASP	C-N-CA	5.30	124.81	119.19
3	H	39	HIS	N-CA-C	5.29	121.55	113.61
1	E	212	PHE	N-CA-C	5.29	119.38	112.13
1	E	503	GLY	N-CA-C	5.28	120.47	114.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	162	ARG	N-CA-C	-5.28	100.13	108.73
3	G	122	ILE	N-CA-C	-5.27	105.94	110.74
2	C	83	TRP	N-CA-C	-5.25	100.14	109.06
1	D	196	ASP	N-CA-C	-5.24	102.64	110.23
2	C	265	PHE	N-CA-C	5.24	116.80	111.14
3	H	74	GLU	N-CA-C	5.24	116.67	111.07
3	G	39	HIS	N-CA-C	5.20	122.11	113.89
1	E	178	GLY	N-CA-C	5.20	122.94	112.34
2	B	153	LEU	CA-CB-CG	5.18	134.44	116.30
3	G	38	ASP	N-CA-C	5.17	117.00	111.36
2	B	105	TRP	N-CA-C	-5.16	101.83	109.94
2	B	137	ASN	CA-C-N	5.16	124.77	119.05
2	B	137	ASN	C-N-CA	5.16	124.77	119.05
1	D	38	ASP	N-CA-C	5.14	117.94	109.76
2	C	134	ARG	N-CA-C	5.14	117.55	111.33
2	C	149	TRP	N-CA-C	-5.13	105.76	111.36
1	E	309	VAL	N-CA-C	5.11	116.20	111.45
2	B	252	TYR	N-CA-C	5.10	116.53	110.97
2	B	145	ILE	CB-CA-C	-5.09	105.30	111.87
1	E	193	ILE	N-CA-C	5.09	119.93	109.34
3	H	73	ASN	N-CA-C	-5.07	103.99	110.53
1	E	188	PHE	N-CA-C	5.07	119.42	112.88
1	E	213	THR	N-CA-C	5.06	117.18	111.11
1	E	104	LYS	N-CA-C	-5.06	105.66	111.07
2	C	268	LEU	N-CA-C	5.04	119.55	113.41

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	299	TYR	Sidechain
1	D	67	TYR	Sidechain
1	E	67	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4186	934	3990	127	1
1	E	4186	934	3990	145	0
2	B	3167	0	3014	93	0
2	C	3167	707	3014	89	0
3	G	1337	321	1323	32	0
3	H	1337	321	1323	35	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
5	B	263	526	0	14	0
5	C	269	538	0	11	0
5	D	292	584	0	23	7
5	E	308	616	0	23	2
5	G	157	314	0	8	2
5	H	199	398	0	11	5
All	All	18872	6193	16654	454	11

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 13.

All (454) 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)
2:C:133:ILE:HG21	2:C:203:ILE:HD12	1.45	0.97
3:G:41:THR:O	3:G:44:ARG:HD2	1.70	0.91
1:E:78:GLN:HE22	1:E:150:GLN:HE21	1.19	0.88
2:C:336:MET:SD	5:C:627:HOH:O	2.32	0.87
1:D:84:VAL:HG21	1:E:77:ARG:HB3	1.55	0.87
2:C:311:ASP:HB2	5:C:636:HOH:O	1.75	0.87
1:D:78:GLN:HE22	1:D:150:GLN:HE21	1.19	0.86
1:E:512:ILE:HA	1:E:515:LEU:HD12	1.56	0.86
1:D:505:LYS:HB2	5:D:707:HOH:O	1.73	0.86
1:D:383:TYR:HB2	5:D:800:HOH:O	1.76	0.84
2:B:136:MET:HE1	2:B:145:ILE:CD1	2.07	0.84
1:D:510:ASP:HB3	5:D:631:HOH:O	1.78	0.84
2:B:136:MET:SD	5:B:534:HOH:O	2.36	0.83
1:D:155:ASN:HD22	1:D:168:HIS:HD2	1.28	0.82
2:C:267:ARG:HH22	2:C:347:THR:HG21	1.46	0.81
1:D:381:ASP:HB2	5:D:720:HOH:O	1.81	0.81
2:B:225:LYS:HA	2:B:225:LYS:CE	2.10	0.80
1:E:16:ALA:HA	2:B:362:ASP:CG	2.06	0.79
2:C:357:TYR:HD1	2:C:377:ARG:HH12	1.29	0.79
2:B:136:MET:HE1	2:B:145:ILE:HD11	1.65	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:MET:HB2	2:C:168:ARG:HD3	1.65	0.78
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.31	0.77
1:E:16:ALA:H	2:B:362:ASP:HB3	1.49	0.77
1:D:84:VAL:CG2	1:E:77:ARG:HB3	2.14	0.77
3:H:41:THR:O	3:H:44:ARG:HD2	1.84	0.77
1:D:83:GLN:HB3	1:E:77:ARG:NH2	1.99	0.77
2:B:261:ARG:HE	2:B:285:GLN:HE22	1.32	0.75
2:C:357:TYR:HD1	2:C:377:ARG:NH1	1.85	0.75
1:D:519:PHE:O	1:D:520:LYS:HE2	1.87	0.74
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.35	0.74
3:H:11:THR:HG21	5:H:415:HOH:O	1.87	0.74
2:B:194:GLN:HE22	2:B:197:ARG:HH11	1.34	0.73
2:B:44:LYS:H	2:B:44:LYS:HD3	1.53	0.73
1:E:269:THR:HG21	5:H:357:HOH:O	1.88	0.73
2:C:100:ASP:OD2	2:C:104:ARG:HD3	1.89	0.73
1:D:360:ARG:HH22	1:D:506:LEU:HD21	1.54	0.72
2:B:221:GLY:O	2:B:225:LYS:HG2	1.89	0.72
2:B:44:LYS:HD3	2:B:44:LYS:N	2.04	0.72
3:G:43:PHE:CZ	3:G:109:LYS:HE2	2.25	0.72
1:E:175:ARG:HD3	1:E:181:TRP:CE2	2.25	0.72
3:H:79:HIS:HD2	3:H:127:TYR:OH	1.72	0.72
2:C:36:GLY:N	5:C:446:HOH:O	2.22	0.71
1:D:384:GLY:N	5:D:800:HOH:O	2.23	0.70
1:D:44:THR:HG22	1:D:46:TYR:H	1.55	0.70
3:G:79:HIS:HD2	3:G:127:TYR:OH	1.75	0.70
2:C:357:TYR:CD1	2:C:377:ARG:NH1	2.60	0.70
1:E:292:TYR:OH	1:E:344:HIS:HD2	1.75	0.70
1:D:24:ASN:OD1	1:D:26:GLN:HG2	1.92	0.69
1:D:352:ALA:HA	1:D:404:PRO:HB2	1.73	0.69
3:G:19:ILE:O	3:G:22:VAL:HG22	1.92	0.68
3:G:138:ARG:HG3	3:G:138:ARG:HH11	1.58	0.68
5:E:786:HOH:O	3:H:165:HIS:HA	1.93	0.68
2:C:258:GLN:HE21	2:C:261:ARG:HH21	1.41	0.68
1:D:493:LYS:HE2	5:D:633:HOH:O	1.93	0.68
2:B:228:ARG:NH2	5:B:626:HOH:O	2.25	0.68
3:G:138:ARG:NH1	3:G:142:LEU:HD11	2.08	0.68
1:E:15:ALA:N	2:B:288:PHE:CE2	2.62	0.68
2:B:136:MET:HE1	2:B:145:ILE:HD12	1.77	0.67
1:E:352:ALA:HA	1:E:404:PRO:HB2	1.77	0.67
1:D:17:ASN:O	1:D:18:ARG:HB2	1.94	0.67
1:D:413:HIS:HD2	1:D:428:SER:OG	1.78	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ARG:HG3	1:E:176:THR:N	2.10	0.67
2:B:146:ASN:HD21	2:B:197:ARG:HH21	1.41	0.67
1:D:493:LYS:NZ	1:D:508:THR:HG23	2.10	0.67
3:H:100:ALA:HB2	5:H:2060:HOH:O	1.94	0.67
1:E:17:ASN:O	1:E:18:ARG:HB2	1.93	0.66
1:E:108:ASN:HD21	1:E:175:ARG:HH21	1.42	0.66
1:D:521:ASN:HB3	1:D:524:LYS:HD3	1.77	0.66
1:D:230:GLU:HB3	5:E:609:HOH:O	1.94	0.66
2:B:349:LYS:HD2	2:B:389:LYS:HE3	1.77	0.66
3:G:4:LEU:N	5:G:251:HOH:O	2.27	0.66
1:D:83:GLN:HB3	1:E:77:ARG:HH21	1.57	0.66
2:C:194:GLN:HE22	2:C:197:ARG:HH11	1.44	0.66
1:E:15:ALA:N	2:B:288:PHE:HE2	1.94	0.66
1:E:44:THR:HG22	1:E:46:TYR:H	1.61	0.66
1:E:15:ALA:HB2	2:B:367:TYR:HE2	1.61	0.65
1:E:227:ASN:HD21	1:E:295:LYS:H	1.45	0.65
1:E:302:VAL:HG13	1:E:376:TYR:HE2	1.61	0.65
1:E:477:GLU:O	1:E:480:GLU:HG2	1.95	0.65
2:B:194:GLN:HE22	2:B:197:ARG:NH1	1.95	0.65
2:B:266:GLN:HE22	2:B:278:PRO:HA	1.61	0.65
2:B:258:GLN:HE21	2:B:261:ARG:HH21	1.45	0.64
1:D:354:TRP:CZ2	1:D:403:ILE:HD11	2.32	0.64
1:E:16:ALA:N	2:B:362:ASP:HB3	2.13	0.64
2:B:145:ILE:HG12	5:B:535:HOH:O	1.97	0.64
1:D:84:VAL:HB	1:E:81:SER:OG	1.98	0.64
1:E:369:MET:HE3	5:E:815:HOH:O	1.97	0.63
2:C:127:TYR:HE1	2:C:133:ILE:HG22	1.63	0.63
1:D:268:ASN:HD21	1:D:327:GLU:H	1.46	0.63
1:E:489:ARG:HD2	1:E:495:LEU:O	1.97	0.63
1:D:16:ALA:CB	2:C:292:LYS:NZ	2.62	0.63
1:D:18:ARG:NH1	2:B:133:ILE:HD11	2.12	0.63
3:H:39:HIS:HD2	5:H:426:HOH:O	1.80	0.63
1:E:16:ALA:HA	2:B:362:ASP:OD2	1.98	0.63
1:D:16:ALA:HB3	2:C:292:LYS:NZ	2.14	0.62
2:C:133:ILE:CG2	2:C:203:ILE:HD12	2.26	0.62
3:H:22:VAL:CG2	3:H:63:LYS:HG2	2.29	0.62
1:D:175:ARG:HG3	1:D:181:TRP:CD2	2.35	0.62
1:D:302:VAL:HG13	1:D:376:TYR:HE2	1.65	0.62
1:E:269:THR:HG23	5:E:542:HOH:O	1.99	0.62
2:B:371:ILE:HG12	5:B:428:HOH:O	1.99	0.62
1:E:78:GLN:NE2	1:E:150:GLN:HE21	1.94	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:HIS:HD2	1:E:428:SER:OG	1.82	0.61
2:B:225:LYS:HD3	2:B:228:ARG:HH21	1.65	0.61
2:B:370:ARG:HD2	5:B:426:HOH:O	2.00	0.61
1:D:292:TYR:OH	1:D:344:HIS:HD2	1.83	0.61
1:E:403:ILE:HG12	1:E:515:LEU:HD22	1.82	0.60
2:B:259:PHE:CE1	2:B:356:LEU:HD13	2.36	0.60
2:C:179:LEU:HG	5:C:432:HOH:O	2.02	0.60
1:E:268:ASN:HD21	1:E:327:GLU:H	1.50	0.60
1:E:269:THR:HB	3:H:148:TYR:CE2	2.37	0.60
3:G:26:GLU:HG2	5:G:322:HOH:O	2.01	0.60
2:B:371:ILE:HG23	5:B:428:HOH:O	2.01	0.60
1:E:63:ILE:HG22	5:C:500:HOH:O	2.00	0.60
3:G:101:ALA:HB3	3:G:138:ARG:HH12	1.66	0.60
2:C:336:MET:HE3	2:C:388:LEU:HD22	1.85	0.59
1:E:213:THR:O	1:E:217:ILE:HG12	2.01	0.59
1:E:439:HIS:HE1	1:E:454:GLU:OE2	1.85	0.59
1:D:354:TRP:CE2	1:D:403:ILE:HD11	2.38	0.59
1:D:493:LYS:NZ	1:D:510:ASP:H	2.01	0.59
3:G:59:LYS:HG2	5:G:197:HOH:O	2.02	0.59
1:E:175:ARG:HD3	1:E:181:TRP:CZ2	2.37	0.59
2:B:341:LYS:HB3	5:B:647:HOH:O	2.03	0.59
1:D:502:ARG:HD2	5:D:706:HOH:O	2.03	0.58
3:G:44:ARG:HD3	3:G:47:TYR:CZ	2.38	0.58
1:D:379:TRP:CD2	5:D:800:HOH:O	2.52	0.58
1:E:18:ARG:NE	5:E:527:HOH:O	2.37	0.58
2:B:136:MET:HE3	2:B:274:ASP:HB2	1.86	0.58
2:B:161:ASN:HB3	2:B:235:TRP:CE2	2.38	0.58
2:B:349:LYS:CE	2:B:389:LYS:HE3	2.34	0.58
2:C:168:ARG:NE	5:C:433:HOH:O	2.36	0.58
2:C:108:PRO:HA	2:C:111:LYS:HE3	1.85	0.57
1:D:439:HIS:HE1	1:D:454:GLU:OE2	1.87	0.57
2:B:96:PHE:O	2:B:99:ARG:NH2	2.38	0.57
2:B:133:ILE:HG12	5:B:532:HOH:O	2.03	0.57
3:G:33:LYS:HE2	5:G:283:HOH:O	2.04	0.57
3:G:39:HIS:HD2	5:G:237:HOH:O	1.88	0.57
1:D:344:HIS:HE1	1:D:376:TYR:CD2	2.23	0.57
1:D:360:ARG:HH22	1:D:506:LEU:CD2	2.17	0.57
2:B:136:MET:HE2	2:B:140:TRP:HD1	1.70	0.57
1:D:175:ARG:HG2	1:D:176:THR:N	2.17	0.57
1:D:108:ASN:HD21	1:D:175:ARG:HH21	1.53	0.57
1:E:269:THR:HB	3:H:148:TYR:HE2	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:336:MET:HB3	2:C:388:LEU:HA	1.87	0.57
3:H:98:MET:O	3:H:138:ARG:NH1	2.38	0.56
1:D:202:LEU:HD23	1:D:206:LEU:HD23	1.86	0.56
1:E:140:GLN:O	1:E:144:GLU:HG2	2.06	0.56
1:E:123:MET:HE1	1:E:200:CYS:SG	2.45	0.56
2:B:388:LEU:CG	2:B:389:LYS:HD3	2.36	0.56
2:B:225:LYS:HA	2:B:225:LYS:HE3	1.84	0.56
1:E:435:THR:HG23	1:E:449:SER:O	2.05	0.56
3:H:19:ILE:HG12	3:H:60:LEU:HD13	1.86	0.56
3:H:15:TRP:HA	3:H:18:LYS:HG2	1.86	0.56
1:E:15:ALA:HB3	5:B:550:HOH:O	2.05	0.56
1:E:169:ASN:O	2:C:35:MET:O	2.24	0.56
3:H:22:VAL:HG21	3:H:63:LYS:HG2	1.86	0.56
1:D:436:LEU:HD21	1:D:447:THR:HG23	1.87	0.55
1:E:445:MET:HE3	1:E:523:VAL:HG13	1.86	0.55
2:C:179:LEU:HD12	2:C:182:TRP:CE3	2.42	0.55
1:E:88:ARG:NH1	5:E:609:HOH:O	2.38	0.55
2:B:225:LYS:CD	2:B:228:ARG:HH21	2.19	0.55
1:E:40:LYS:HE2	1:E:41:ASN:ND2	2.22	0.55
1:D:77:ARG:HD3	1:E:84:VAL:HG22	1.89	0.55
1:E:33:GLN:HE21	1:E:33:GLN:HA	1.72	0.55
2:B:61:ASP:OD2	3:G:7:HIS:HD2	1.90	0.55
5:B:580:HOH:O	3:G:124:PRO:HA	2.06	0.55
2:C:141:ARG:HA	2:C:145:ILE:HD12	1.88	0.55
1:E:302:VAL:HG13	1:E:376:TYR:CE2	2.42	0.54
2:C:133:ILE:HB	5:C:402:HOH:O	2.07	0.54
3:G:43:PHE:CE1	3:G:109:LYS:HE2	2.42	0.54
1:D:204:LEU:HB2	5:D:770:HOH:O	2.07	0.54
1:E:44:THR:CG2	1:E:127:SER:HA	2.37	0.54
1:E:401:GLY:HA2	1:E:514:ARG:NE	2.22	0.54
1:D:302:VAL:HG13	1:D:376:TYR:CE2	2.42	0.54
1:D:508:THR:HG22	1:D:511:ASP:H	1.71	0.54
1:E:54:ASN:O	1:E:55:GLU:HB2	2.07	0.54
3:G:138:ARG:HH11	3:G:138:ARG:CG	2.20	0.54
1:E:448:PHE:HD1	5:E:567:HOH:O	1.91	0.54
2:B:26:GLU:CD	2:B:26:GLU:H	2.14	0.54
3:H:102:LYS:HD3	5:H:2062:HOH:O	2.07	0.54
1:D:360:ARG:HE	1:D:489:ARG:NH2	2.06	0.54
1:E:369:MET:HE2	1:E:384:GLY:HA2	1.90	0.54
3:H:4:LEU:HG	3:H:10:ASP:H	1.73	0.54
1:E:110:LEU:O	1:E:114:GLU:HG2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:267:ARG:HH22	2:C:347:THR:CG2	2.20	0.53
2:B:376:ASP:HB3	2:B:379:GLN:HB3	1.90	0.53
3:G:79:HIS:HE1	5:G:269:HOH:O	1.90	0.53
1:D:493:LYS:CE	1:D:508:THR:HG23	2.39	0.53
1:E:134:LYS:HD3	2:C:161:ASN:HD21	1.73	0.53
1:E:219:ALA:HA	1:E:222:GLU:CD	2.32	0.53
2:C:333:ARG:HG2	2:C:333:ARG:HH11	1.73	0.53
1:E:33:GLN:HE22	1:E:132:GLU:H	1.56	0.53
2:C:194:GLN:HE22	2:C:197:ARG:NH1	2.06	0.53
2:B:378:ASP:O	2:B:382:LYS:HG2	2.09	0.53
1:D:78:GLN:NE2	1:D:150:GLN:HE21	1.98	0.53
1:D:84:VAL:HG12	1:D:88:ARG:NH2	2.24	0.53
1:D:230:GLU:C	1:D:233:PRO:HD2	2.34	0.53
1:E:169:ASN:HA	2:C:35:MET:HA	1.91	0.53
3:G:154:GLU:HA	3:G:157:LYS:HD3	1.91	0.53
2:B:118:ARG:NH2	2:C:111:LYS:HD2	2.24	0.53
2:C:170:ALA:O	2:C:176:ARG:NH2	2.42	0.52
2:C:336:MET:HE2	2:C:384:VAL:HG12	1.90	0.52
1:D:81:SER:OG	1:E:84:VAL:HB	2.08	0.52
2:C:336:MET:CE	2:C:356:LEU:HD21	2.40	0.52
2:B:349:LYS:CD	2:B:389:LYS:HE3	2.38	0.52
1:D:77:ARG:HB3	1:E:84:VAL:HG21	1.91	0.52
2:C:168:ARG:CZ	5:C:433:HOH:O	2.56	0.52
3:H:41:THR:O	3:H:44:ARG:CD	2.55	0.52
3:H:138:ARG:NH2	5:H:368:HOH:O	2.42	0.52
1:E:523:VAL:HG12	5:E:788:HOH:O	2.10	0.52
2:B:388:LEU:HG	2:B:389:LYS:HD3	1.91	0.52
2:C:98:HIS:HE1	2:C:178:SER:OG	1.93	0.52
3:H:15:TRP:HA	3:H:18:LYS:CG	2.39	0.52
1:D:16:ALA:HA	2:B:129:ALA:O	2.10	0.52
1:E:438:VAL:HB	3:H:164:VAL:HG22	1.91	0.52
2:C:376:ASP:HB3	2:C:379:GLN:HB3	1.92	0.52
1:E:17:ASN:HD21	2:C:134:ARG:NH1	2.08	0.51
1:D:214:ASN:HB3	1:D:215:PRO:HD3	1.92	0.51
1:E:15:ALA:HB2	2:B:367:TYR:CE2	2.44	0.51
2:B:333:ARG:HD3	5:B:399:HOH:O	2.09	0.51
1:D:268:ASN:CG	1:D:327:GLU:HG2	2.36	0.51
1:D:416:TYR:HB3	1:D:447:THR:HG21	1.92	0.51
2:C:168:ARG:NH2	5:C:433:HOH:O	2.43	0.51
1:E:33:GLN:NE2	1:E:132:GLU:H	2.08	0.51
1:E:244:LEU:HB3	5:E:701:HOH:O	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:HG22	1:E:77:ARG:NH1	2.25	0.51
1:D:108:ASN:ND2	1:D:175:ARG:HH21	2.09	0.51
2:C:233:GLY:HA2	2:C:237:GLU:HG2	1.91	0.51
1:D:493:LYS:HZ1	1:D:510:ASP:H	1.58	0.51
2:C:150:GLY:O	2:C:153:LEU:HB3	2.11	0.51
1:E:18:ARG:HH22	2:C:134:ARG:HG3	1.76	0.51
1:E:512:ILE:HA	1:E:515:LEU:CD1	2.34	0.51
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.92	0.51
1:E:108:ASN:ND2	1:E:175:ARG:HH21	2.09	0.50
1:D:268:ASN:ND2	1:D:327:GLU:H	2.09	0.50
1:E:63:ILE:HG23	2:C:191:GLN:CD	2.37	0.50
1:D:77:ARG:HD2	5:D:783:HOH:O	2.12	0.50
1:D:381:ASP:HA	1:D:385:LYS:HD3	1.94	0.50
1:E:380:TYR:CE2	1:E:385:LYS:HD3	2.46	0.50
1:E:524:LYS:N	5:E:788:HOH:O	2.44	0.50
2:B:319:ASN:OD1	3:G:78:ARG:HD3	2.12	0.50
1:E:260:ASP:HB3	5:E:745:HOH:O	2.10	0.50
1:E:511:ASP:O	1:E:514:ARG:HG3	2.11	0.50
2:C:374:LYS:HG3	2:C:374:LYS:O	2.11	0.50
2:C:259:PHE:CE1	2:C:356:LEU:HD13	2.46	0.50
2:C:22:LYS:HE2	2:C:23:ALA:N	2.27	0.50
5:D:785:HOH:O	2:B:106:HIS:CE1	2.65	0.49
5:E:785:HOH:O	3:H:165:HIS:HA	2.12	0.49
2:B:98:HIS:HE1	2:B:178:SER:OG	1.95	0.49
2:C:336:MET:HE1	2:C:356:LEU:HD21	1.93	0.49
2:C:22:LYS:HE2	2:C:22:LYS:C	2.37	0.49
3:H:79:HIS:CD2	3:H:127:TYR:OH	2.61	0.49
1:E:227:ASN:ND2	1:E:295:LYS:H	2.08	0.49
2:B:100:ASP:OD2	2:B:104:ARG:HG2	2.11	0.49
1:D:16:ALA:HB3	2:C:292:LYS:HZ2	1.76	0.49
2:C:361:ASP:O	2:C:365:GLU:HG2	2.11	0.49
1:D:212:PHE:O	1:D:215:PRO:HD2	2.13	0.49
1:D:16:ALA:HB2	2:C:292:LYS:NZ	2.28	0.49
1:D:313:TRP:HA	1:D:317:TRP:HB3	1.94	0.49
1:E:18:ARG:HH22	2:C:134:ARG:CG	2.26	0.49
1:E:18:ARG:NH1	2:C:133:ILE:HD11	2.28	0.49
1:D:281:TYR:CZ	1:D:285:VAL:HG21	2.48	0.49
1:E:164:ASP:OD1	1:E:489:ARG:NH2	2.46	0.49
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.47	0.49
1:D:413:HIS:CD2	1:D:428:SER:OG	2.64	0.48
1:E:171:ALA:O	1:E:175:ARG:HG2	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:LYS:HE3	2:B:225:LYS:CA	2.43	0.48
3:G:44:ARG:HG3	3:G:46:SER:O	2.13	0.48
3:G:109:LYS:HE3	5:G:300:HOH:O	2.13	0.48
1:E:84:VAL:HG12	1:E:88:ARG:NH2	2.28	0.48
2:C:34:LYS:O	2:C:35:MET:O	2.32	0.48
1:D:379:TRP:CE3	5:D:800:HOH:O	2.67	0.48
1:D:493:LYS:HZ1	1:D:508:THR:HG23	1.77	0.48
1:D:140:GLN:O	1:D:144:GLU:HG2	2.13	0.48
2:B:370:ARG:HB2	5:B:428:HOH:O	2.13	0.48
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.95	0.47
1:E:123:MET:SD	2:C:168:ARG:NH1	2.87	0.47
2:C:361:ASP:OD1	2:C:377:ARG:NH1	2.48	0.47
1:D:134:LYS:HD3	2:B:161:ASN:HD21	1.79	0.47
1:E:292:TYR:OH	1:E:344:HIS:CD2	2.63	0.47
5:E:786:HOH:O	3:H:165:HIS:CD2	2.67	0.47
3:H:20:ALA:HB3	5:H:409:HOH:O	2.14	0.47
2:C:240:ASP:HB2	3:H:125:VAL:CG2	2.45	0.47
1:D:30:ARG:HD2	1:D:31:TRP:NE1	2.29	0.47
1:E:519:PHE:C	1:E:520:LYS:HD2	2.40	0.47
2:B:364:ILE:HA	2:B:368:ALA:HB3	1.97	0.47
1:D:108:ASN:HD21	1:D:175:ARG:HE	1.62	0.47
2:B:6:GLU:HG2	2:B:7:ARG:N	2.29	0.47
2:C:269:ALA:N	2:C:270:PRO:CD	2.78	0.47
1:D:217:ILE:HG13	5:D:642:HOH:O	2.14	0.47
1:D:500:HIS:NE2	5:D:707:HOH:O	2.35	0.47
1:E:401:GLY:C	1:E:515:LEU:HD23	2.40	0.47
2:C:133:ILE:HG13	2:C:134:ARG:N	2.30	0.47
1:D:360:ARG:NH1	2:B:29:LEU:HG	2.29	0.47
1:E:15:ALA:O	1:E:16:ALA:HB3	2.15	0.47
1:E:15:ALA:HB1	2:B:362:ASP:O	2.15	0.46
1:D:436:LEU:CD2	1:D:447:THR:HG23	2.45	0.46
1:D:227:ASN:HD21	1:D:296:PHE:H	1.62	0.46
1:D:160:LYS:NZ	1:D:161:ASN:HD21	2.14	0.46
1:D:227:ASN:HD21	1:D:295:LYS:H	1.63	0.46
1:E:209:GLU:HA	1:E:213:THR:HB	1.97	0.46
1:D:175:ARG:HG3	1:D:181:TRP:CE2	2.51	0.46
1:E:101:GLU:CD	1:E:360:ARG:HD3	2.41	0.46
2:B:42:ARG:HB2	2:B:99:ARG:HG3	1.97	0.46
2:B:225:LYS:CE	2:B:225:LYS:CA	2.88	0.46
2:B:225:LYS:HG3	5:B:628:HOH:O	2.15	0.46
1:D:76:GLU:HG3	5:D:670:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:GLY:HA2	1:E:514:ARG:HE	1.80	0.46
2:C:44:LYS:HA	2:C:44:LYS:HD3	1.68	0.46
1:E:223:TRP:CZ3	1:E:297:LYS:HA	2.50	0.46
1:E:427:PRO:HD2	5:E:646:HOH:O	2.15	0.46
1:D:84:VAL:HG12	1:D:88:ARG:HH21	1.80	0.46
1:E:437:ARG:HA	5:E:786:HOH:O	2.16	0.46
1:E:493:LYS:HB2	1:E:493:LYS:NZ	2.30	0.46
2:B:270:PRO:HB3	2:C:270:PRO:HB3	1.98	0.46
1:E:110:LEU:HD23	1:E:151:CYS:SG	2.56	0.46
1:D:147:HIS:CE1	5:D:639:HOH:O	2.69	0.45
2:C:159:LEU:HG	2:C:248:VAL:HG13	1.98	0.45
1:D:16:ALA:CB	2:B:129:ALA:O	2.64	0.45
1:D:292:TYR:OH	1:D:344:HIS:CD2	2.67	0.45
1:D:366:GLN:O	1:D:370:GLU:HG3	2.17	0.45
1:D:500:HIS:CE1	5:D:707:HOH:O	2.69	0.45
2:B:33:ASN:HD22	2:B:33:ASN:H	1.64	0.45
2:C:61:ASP:OD2	3:H:7:HIS:HD2	1.98	0.45
2:C:111:LYS:O	2:C:115:GLU:HG3	2.16	0.45
1:D:169:ASN:HD22	1:D:170:ASP:N	2.14	0.45
1:E:252:GLN:HG2	5:E:740:HOH:O	2.16	0.45
1:D:398:PRO:HG3	1:D:507:TRP:CD1	2.52	0.45
1:E:30:ARG:HG3	5:E:825:HOH:O	2.16	0.45
2:B:44:LYS:HE2	2:B:45:ARG:NH2	2.31	0.45
2:B:349:LYS:HE2	5:B:438:HOH:O	2.16	0.45
2:B:388:LEU:HB3	2:B:389:LYS:HZ2	1.82	0.45
2:C:233:GLY:HA2	2:C:237:GLU:CG	2.46	0.45
1:E:164:ASP:CG	1:E:489:ARG:HH22	2.24	0.45
1:E:268:ASN:OD1	1:E:327:GLU:HG2	2.17	0.45
1:E:286:LEU:HG	5:E:536:HOH:O	2.17	0.45
1:E:313:TRP:HA	1:E:317:TRP:HB3	1.98	0.45
2:C:159:LEU:HD23	2:C:186:LYS:HE3	1.98	0.45
1:E:169:ASN:HD22	1:E:170:ASP:N	2.14	0.45
1:E:495:LEU:HD11	1:E:512:ILE:CG1	2.47	0.45
5:E:786:HOH:O	3:H:165:HIS:HD2	1.99	0.45
2:B:78:GLY:O	3:G:115:ARG:HD3	2.17	0.45
2:B:266:GLN:HE21	2:B:266:GLN:HA	1.82	0.45
2:C:89:GLU:CD	3:H:125:VAL:HG13	2.42	0.44
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.00	0.44
1:D:360:ARG:NH1	5:D:615:HOH:O	2.49	0.44
1:E:397:ASP:HA	1:E:398:PRO:HD3	1.91	0.44
2:C:57:GLN:OE1	2:C:176:ARG:NH2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:196:GLU:HG3	2:C:276:LEU:HD13	2.00	0.44
3:H:27:LYS:NZ	5:H:2043:HOH:O	2.50	0.44
1:D:49:LYS:HD3	3:G:144:ASN:HD22	1.82	0.44
1:E:240:GLU:HG3	5:E:772:HOH:O	2.17	0.44
1:E:512:ILE:CA	1:E:515:LEU:HD12	2.39	0.44
1:D:125:TRP:HE1	2:B:161:ASN:ND2	2.16	0.44
1:D:282:PHE:HB3	1:D:286:LEU:HD22	2.00	0.44
1:D:360:ARG:HH21	1:D:489:ARG:CZ	2.31	0.44
2:B:33:ASN:HD22	2:B:33:ASN:N	2.14	0.44
2:C:223:VAL:HG13	2:C:335:PHE:HA	2.00	0.44
1:D:77:ARG:HH11	1:E:84:VAL:HG22	1.82	0.44
1:D:372:PHE:HB3	1:D:379:TRP:CD2	2.53	0.44
1:D:445:MET:HE3	1:D:523:VAL:HG13	2.00	0.44
2:B:194:GLN:NE2	2:B:197:ARG:HH11	2.10	0.44
3:G:21:HIS:CD2	5:G:289:HOH:O	2.71	0.44
3:H:11:THR:HG23	5:H:2711:HOH:O	2.17	0.44
1:E:269:THR:HG22	5:E:712:HOH:O	2.17	0.44
1:E:302:VAL:CG1	1:E:376:TYR:HE2	2.30	0.43
2:B:150:GLY:O	2:B:153:LEU:HB3	2.18	0.43
1:D:65:LYS:HB3	2:B:117:TRP:CG	2.53	0.43
1:E:211:CYS:HB2	1:E:313:TRP:CD1	2.53	0.43
1:D:403:ILE:HD12	5:D:636:HOH:O	2.18	0.43
1:E:15:ALA:O	1:E:16:ALA:CB	2.66	0.43
2:B:258:GLN:NE2	2:B:261:ARG:HH21	2.13	0.43
1:E:40:LYS:HG3	5:E:778:HOH:O	2.18	0.43
1:E:484:GLU:HG2	5:H:2718:HOH:O	2.19	0.43
1:E:488:LEU:HD11	1:E:509:LEU:HD22	2.01	0.43
2:C:377:ARG:HH11	2:C:377:ARG:HB2	1.83	0.43
1:D:244:LEU:HD13	5:D:693:HOH:O	2.19	0.43
1:D:227:ASN:ND2	1:D:295:LYS:H	2.16	0.43
1:D:354:TRP:CG	1:D:355:PRO:HD3	2.53	0.43
1:D:521:ASN:HD22	1:D:524:LYS:HZ3	1.66	0.43
2:C:127:TYR:CE1	2:C:133:ILE:HG22	2.49	0.43
3:G:32:LEU:HD13	3:G:60:LEU:HB3	2.00	0.43
1:E:116:ASN:CG	1:E:189:SER:HA	2.44	0.43
2:C:339:PHE:HA	2:C:342:LEU:HD22	1.99	0.43
1:D:188:PHE:CD1	1:D:192:PHE:CZ	3.07	0.43
1:D:360:ARG:NH2	1:D:506:LEU:HG	2.34	0.43
1:D:466:CYS:HB2	2:B:73:THR:HA	2.00	0.43
2:B:44:LYS:NZ	2:B:45:ARG:H	2.17	0.43
3:H:165:HIS:HB3	5:H:1482:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:HIS:ND1	1:E:61:LYS:HG3	2.34	0.42
1:E:230:GLU:OE2	2:C:9:ARG:HD3	2.19	0.42
2:B:146:ASN:ND2	2:B:197:ARG:HH21	2.12	0.42
3:G:153:GLU:CD	3:G:153:GLU:H	2.28	0.42
1:D:76:GLU:HB3	1:E:76:GLU:OE2	2.20	0.42
1:D:165:PRO:HG3	5:D:803:HOH:O	2.18	0.42
1:D:268:ASN:ND2	1:D:327:GLU:HG2	2.33	0.42
1:E:63:ILE:HG23	2:C:191:GLN:OE1	2.20	0.42
1:E:165:PRO:HG2	2:C:30:ASP:HB3	2.00	0.42
1:E:281:TYR:CZ	1:E:285:VAL:HG21	2.55	0.42
2:C:111:LYS:HD3	5:C:459:HOH:O	2.19	0.42
1:E:439:HIS:CE1	1:E:454:GLU:OE2	2.70	0.42
1:D:397:ASP:HA	1:D:398:PRO:HD3	1.92	0.42
1:E:17:ASN:HB3	2:B:365:GLU:OE1	2.20	0.42
1:E:175:ARG:HD2	5:C:449:HOH:O	2.19	0.42
1:E:493:LYS:NZ	1:E:493:LYS:CB	2.83	0.42
2:B:357:TYR:CD1	2:B:377:ARG:NH1	2.87	0.42
1:D:171:ALA:O	1:D:175:ARG:HB3	2.20	0.42
1:E:18:ARG:NH2	2:C:134:ARG:HG3	2.35	0.42
1:D:360:ARG:NE	1:D:489:ARG:NH2	2.67	0.41
1:E:196:ASP:HB2	3:H:140:MET:SD	2.59	0.41
1:E:123:MET:HE3	1:E:197:ALA:HA	2.02	0.41
2:B:136:MET:CE	2:B:140:TRP:HD1	2.32	0.41
3:H:94:THR:HG21	3:H:114:PHE:CD1	2.55	0.41
1:D:495:LEU:HD11	1:D:512:ILE:HG13	2.02	0.41
1:E:489:ARG:NH2	2:C:29:LEU:HB3	2.36	0.41
2:B:389:LYS:HE2	2:B:389:LYS:HB2	1.70	0.41
1:D:343:HIS:CD2	1:D:343:HIS:H	2.38	0.41
1:E:186:ARG:HA	2:C:73:THR:OG1	2.20	0.41
2:C:80:ARG:HD2	2:C:81:PRO:O	2.20	0.41
3:H:22:VAL:HG22	3:H:63:LYS:NZ	2.36	0.41
3:H:57:GLU:O	3:H:61:GLU:HG3	2.21	0.41
1:E:78:GLN:HE21	1:E:235:VAL:HA	1.85	0.41
1:E:215:PRO:HB2	1:E:308:TRP:CE2	2.56	0.41
3:G:22:VAL:CG2	3:G:63:LYS:HG2	2.51	0.41
1:D:493:LYS:HD2	5:D:732:HOH:O	2.20	0.41
1:E:286:LEU:HA	1:E:286:LEU:HD13	1.69	0.41
1:D:360:ARG:HH12	2:B:29:LEU:HG	1.84	0.41
1:D:425:PHE:HZ	1:D:447:THR:HG22	1.86	0.41
1:E:268:ASN:CG	1:E:327:GLU:HG2	2.46	0.41
1:D:354:TRP:NE1	1:D:403:ILE:HD11	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:HIS:CE1	5:E:584:HOH:O	2.74	0.41
1:E:169:ASN:CA	2:C:35:MET:HA	2.51	0.41
1:E:207:VAL:HG11	1:E:275:PHE:HA	2.02	0.41
1:D:78:GLN:O	1:D:82:LEU:HD22	2.21	0.41
1:D:108:ASN:HD21	1:D:175:ARG:NH2	2.16	0.41
1:E:15:ALA:N	2:B:288:PHE:CZ	2.88	0.41
3:G:79:HIS:CD2	3:G:127:TYR:OH	2.64	0.41
3:H:55:TRP:CZ2	3:H:59:LYS:HE2	2.56	0.41
1:D:163:GLN:O	2:B:28:PRO:HA	2.21	0.40
2:B:263:GLU:HB3	2:B:355:SER:HB2	2.02	0.40
2:B:357:TYR:OH	2:B:382:LYS:NZ	2.51	0.40
1:D:90:ASN:HD22	1:D:90:ASN:HA	1.75	0.40
1:D:204:LEU:HG	1:D:205:GLN:HG3	2.03	0.40
3:G:17:ASN:OD1	3:G:21:HIS:HE1	2.04	0.40
1:D:472:GLN:NE2	5:D:663:HOH:O	2.55	0.40
1:E:60:PHE:HZ	1:E:244:LEU:HD11	1.87	0.40
1:E:459:ALA:C	1:E:460:GLU:HG3	2.46	0.40
1:E:514:ARG:HE	1:E:515:LEU:HG	1.86	0.40
2:B:235:TRP:CD1	2:B:235:TRP:C	2.99	0.40
3:G:32:LEU:HA	3:G:60:LEU:HD13	2.03	0.40
3:G:120:PRO:HD3	3:G:128:PHE:CG	2.56	0.40
1:E:15:ALA:HB1	2:B:362:ASP:C	2.46	0.40
2:B:269:ALA:N	2:B:270:PRO:CD	2.84	0.40
2:C:34:LYS:O	2:C:35:MET:C	2.65	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:ARG:HE	5:D:760:HOH:H2[3_755]	1.26	0.34
5:D:720:HOH:O	5:E:813:HOH:H2[3_645]	1.48	0.12
5:H:2509:HOH:O	5:H:2644:HOH:H2[4_565]	1.48	0.12
5:H:2506:HOH:O	5:H:2640:HOH:H1[4_565]	1.51	0.09
5:H:2509:HOH:H2	5:H:2638:HOH:O[4_565]	1.53	0.07
5:D:700:HOH:H2	5:G:256:HOH:O[1_455]	1.56	0.04
5:D:696:HOH:O	5:G:254:HOH:H1[1_455]	1.57	0.03
5:D:817:HOH:O	5:H:2729:HOH:H1[1_545]	1.57	0.03
5:D:528:HOH:O	5:D:707:HOH:H2[3_745]	1.58	0.02
5:D:528:HOH:H1	5:D:637:HOH:O[3_745]	1.59	0.01
5:E:538:HOH:H1	5:H:408:HOH:O[1_655]	1.59	0.01

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	D	510/512 (100%)	491 (96%)	17 (3%)	2 (0%)	30	16
1	E	510/512 (100%)	489 (96%)	16 (3%)	5 (1%)	12	3
2	B	382/384 (100%)	369 (97%)	12 (3%)	1 (0%)	36	22
2	C	382/384 (100%)	369 (97%)	9 (2%)	4 (1%)	12	3
3	G	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
3	H	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
All	All	2104/2116 (99%)	2034 (97%)	58 (3%)	12 (1%)	21	9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	18	ARG
1	E	16	ALA
1	E	18	ARG
2	C	35	MET
1	E	433	ALA
1	E	434	SER
2	C	36	GLY
2	C	64	ALA
1	D	84	VAL
2	B	251	VAL
1	E	84	VAL
2	C	251	VAL

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	432/432 (100%)	405 (94%)	27 (6%)	16	5
1	E	432/432 (100%)	407 (94%)	25 (6%)	18	5
2	B	319/319 (100%)	300 (94%)	19 (6%)	17	5
2	C	319/319 (100%)	300 (94%)	19 (6%)	17	5
3	G	140/140 (100%)	131 (94%)	9 (6%)	16	4
3	H	140/140 (100%)	132 (94%)	8 (6%)	18	6
All	All	1782/1782 (100%)	1675 (94%)	107 (6%)	17	5

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	18	ARG
1	D	59	GLN
1	D	82	LEU
1	D	89	LEU
1	D	125	TRP
1	D	169	ASN
1	D	175	ARG
1	D	260	ASP
1	D	271	LEU
1	D	279	GLN
1	D	286	LEU
1	D	289	LEU
1	D	310	TYR
1	D	332	LEU
1	D	346	LEU
1	D	349	LEU
1	D	361	LEU
1	D	403	ILE
1	D	436	LEU
1	D	437	ARG
1	D	478	LEU
1	D	488	LEU
1	D	506	LEU
1	D	508	THR
1	D	509	LEU
1	D	520	LYS
1	D	523	VAL
1	E	17	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	18	ARG
1	E	51	LYS
1	E	112	VAL
1	E	138	LEU
1	E	169	ASN
1	E	204	LEU
1	E	240	GLU
1	E	244	LEU
1	E	263	SER
1	E	269	THR
1	E	271	LEU
1	E	279	GLN
1	E	286	LEU
1	E	289	LEU
1	E	332	LEU
1	E	346	LEU
1	E	429	LEU
1	E	436	LEU
1	E	458	LEU
1	E	469	ILE
1	E	474	GLU
1	E	493	LYS
1	E	514	ARG
1	E	524	LYS
2	B	21	LEU
2	B	29	LEU
2	B	33	ASN
2	B	44	LYS
2	B	67	LEU
2	B	93	VAL
2	B	133	ILE
2	B	153	LEU
2	B	159	LEU
2	B	168	ARG
2	B	171	LEU
2	B	173	ASP
2	B	179	LEU
2	B	225	LYS
2	B	229	LEU
2	B	266	GLN
2	B	303	LEU
2	B	356	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	389	LYS
2	C	11	LEU
2	C	21	LEU
2	C	22	LYS
2	C	35	MET
2	C	80	ARG
2	C	153	LEU
2	C	159	LEU
2	C	171	LEU
2	C	173	ASP
2	C	225	LYS
2	C	276	LEU
2	C	303	LEU
2	C	308	GLU
2	C	333	ARG
2	C	342	LEU
2	C	347	THR
2	C	356	LEU
2	C	377	ARG
2	C	388	LEU
3	G	25	LEU
3	G	44	ARG
3	G	60	LEU
3	G	102	LYS
3	G	125	VAL
3	G	135	LEU
3	G	138	ARG
3	G	161	VAL
3	G	162	ARG
3	H	11	THR
3	H	16	VAL
3	H	25	LEU
3	H	44	ARG
3	H	60	LEU
3	H	91	LEU
3	H	125	VAL
3	H	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	41	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	78	GLN
1	D	90	ASN
1	D	100	ASN
1	D	108	ASN
1	D	133	GLN
1	D	161	ASN
1	D	168	HIS
1	D	169	ASN
1	D	203	ASN
1	D	227	ASN
1	D	249	ASN
1	D	268	ASN
1	D	273	ASN
1	D	279	GLN
1	D	337	GLN
1	D	343	HIS
1	D	344	HIS
1	D	413	HIS
1	D	422	GLN
1	D	439	HIS
1	D	472	GLN
1	D	486	HIS
1	D	521	ASN
1	E	17	ASN
1	E	59	GLN
1	E	78	GLN
1	E	90	ASN
1	E	108	ASN
1	E	133	GLN
1	E	161	ASN
1	E	168	HIS
1	E	169	ASN
1	E	203	ASN
1	E	227	ASN
1	E	249	ASN
1	E	259	ASN
1	E	268	ASN
1	E	273	ASN
1	E	279	GLN
1	E	343	HIS
1	E	344	HIS
1	E	411	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	412	ASN
1	E	413	HIS
1	E	422	GLN
1	E	439	HIS
1	E	442	ASN
1	E	451	GLN
1	E	472	GLN
1	E	486	HIS
2	B	33	ASN
2	B	98	HIS
2	B	146	ASN
2	B	161	ASN
2	B	194	GLN
2	B	258	GLN
2	B	266	GLN
2	B	283	GLN
2	B	285	GLN
2	B	301	ASN
2	C	98	HIS
2	C	161	ASN
2	C	194	GLN
2	C	258	GLN
2	C	283	GLN
2	C	285	GLN
3	G	7	HIS
3	G	21	HIS
3	G	39	HIS
3	G	45	ASN
3	G	79	HIS
3	G	134	GLN
3	G	144	ASN
3	G	165	HIS
3	H	39	HIS
3	H	45	ASN
3	H	79	HIS
3	H	134	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.