



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:05 AM UTC

PDB ID : 1DCP / pdb_00001dcp
Title : DCOH, A BIFUNCTIONAL PROTEIN-BINDING TRANSCRIPTIONAL COACTIVATOR, COMPLEXED WITH BIOPTERIN
Authors : Cronk, J.D.; Endrizzi, J.A.; Alber, T.
Deposited on : 1996-05-16
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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

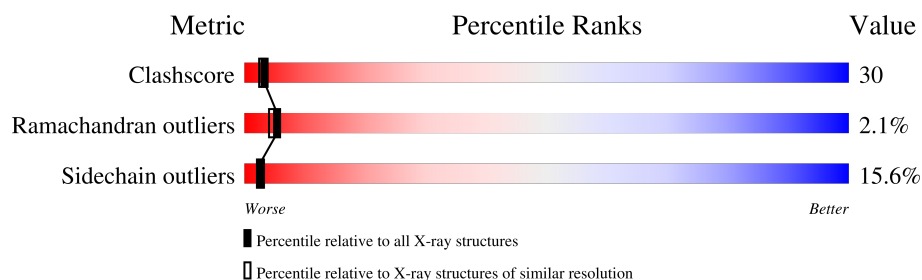
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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	A	104	38% 40% 15% • 5%
1	B	104	37% 41% 14% • 5%
1	C	104	29% 54% 12% • 5%
1	D	104	33% 47% 13% • 5%
1	E	104	43% 36% 14% • 5%
1	F	104	47% 40% 8% 5%
1	G	104	51% 38% 5% • 5%
1	H	104	49% 31% 14% • 5%

2 Entry composition

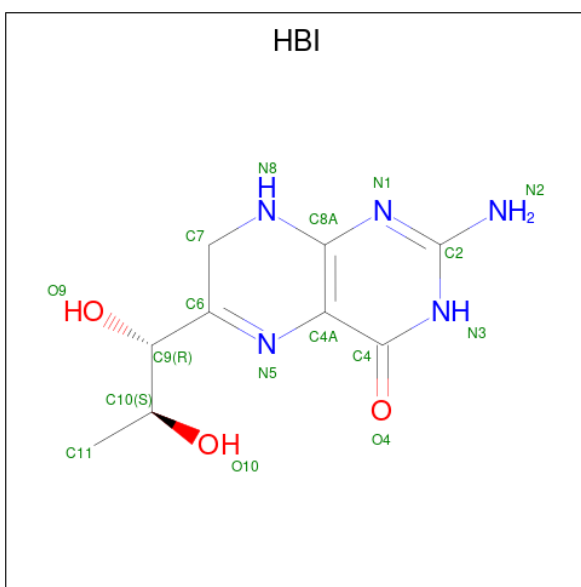
There are 3 unique types of molecules in this entry. The entry contains 6881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DCOH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			811	515	147	146	3			
1	B	99	Total	C	N	O	S	0	0	0
			811	515	147	146	3			
1	C	99	Total	C	N	O	S	0	0	0
			815	517	148	147	3			
1	D	99	Total	C	N	O	S	0	0	0
			812	516	148	145	3			
1	E	99	Total	C	N	O	S	0	0	0
			806	512	146	145	3			
1	F	99	Total	C	N	O	S	0	0	0
			812	516	148	145	3			
1	G	99	Total	C	N	O	S	0	0	0
			810	514	146	147	3			
1	H	99	Total	C	N	O	S	0	0	0
			810	514	146	147	3			

- Molecule 2 is 7,8-DIHYDROBIOPTERIN (CCD ID: HBI) (formula: $C_9H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 17	C 9	N 5	O 3	0	0
2	B	1	Total 17	C 9	N 5	O 3	0	0
2	C	1	Total 17	C 9	N 5	O 3	0	0
2	D	1	Total 17	C 9	N 5	O 3	0	0
2	E	1	Total 17	C 9	N 5	O 3	0	0
2	F	1	Total 17	C 9	N 5	O 3	0	0
2	G	1	Total 17	C 9	N 5	O 3	0	0
2	H	1	Total 17	C 9	N 5	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	35	Total O 35 35	0	0
3	B	31	Total O 31 31	0	0
3	C	36	Total O 36 36	0	0
3	D	27	Total O 27 27	0	0

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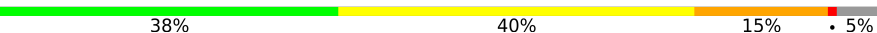
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	28	Total 28	O 28	0	0
3	F	27	Total 27	O 27	0	0
3	G	41	Total 41	O 41	0	0
3	H	33	Total 33	O 33	0	0

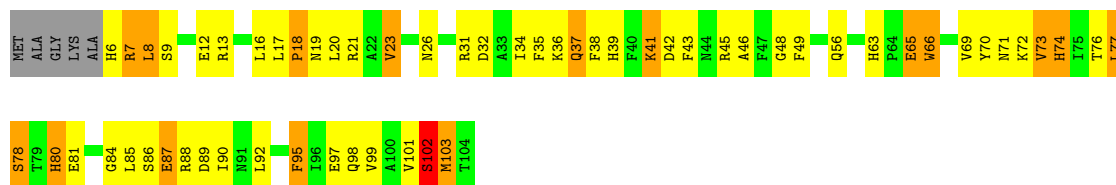
3 Residue-property plots

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

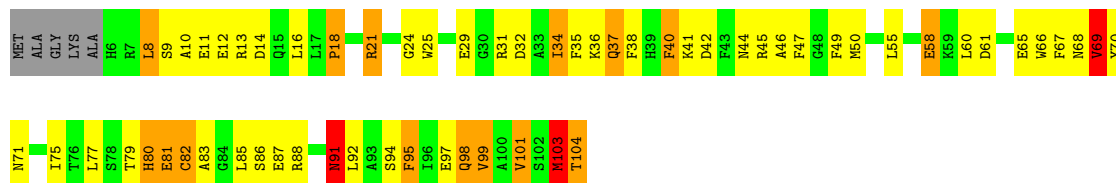
• Molecule 1: DCOH

Chain A: 



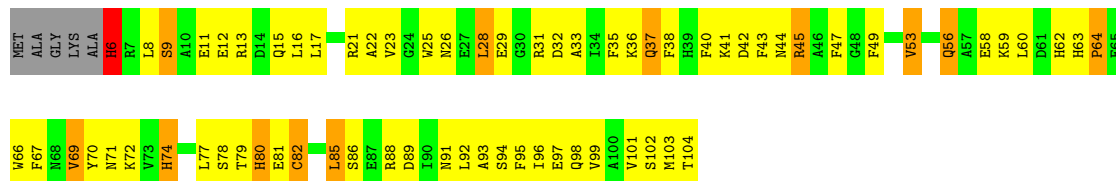
• Molecule 1: DCOH

Chain B: 



• Molecule 1: DCOH

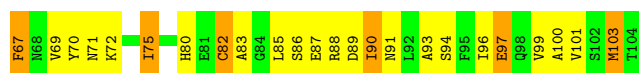
Chain C: 



• Molecule 1: DCOH

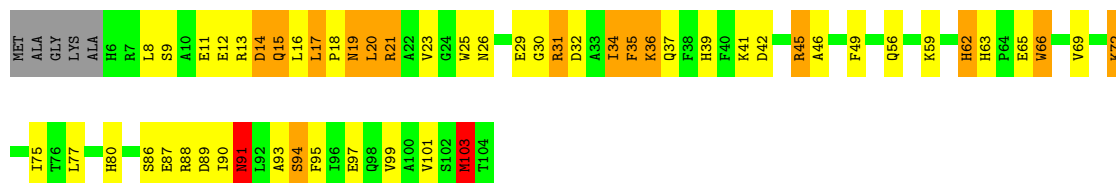
Chain D: 





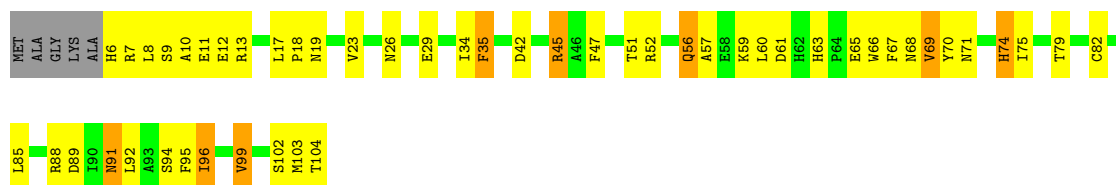
• Molecule 1: DCOH

Chain E: 43% 36% 14% 5%



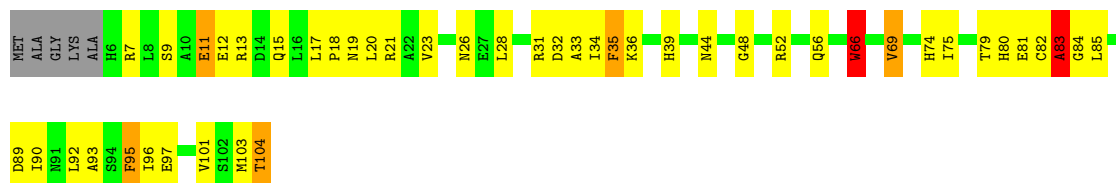
• Molecule 1: DCOH

Chain F: 47% 40% 8% 5%



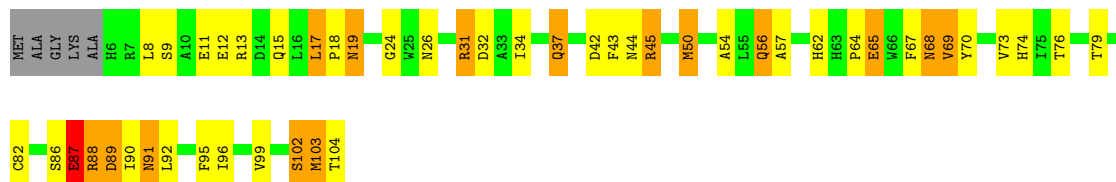
• Molecule 1: DCOH

Chain G: 51% 38% 5% 5%



• Molecule 1: DCOH

Chain H: 49% 31% 14% 5%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	105.70Å 105.70Å 196.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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: HBI

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	1.09	0/831	1.67	9/1122 (0.8%)
1	B	1.16	0/831	1.74	14/1122 (1.2%)
1	C	1.09	0/835	1.73	11/1127 (1.0%)
1	D	1.16	1/832 (0.1%)	1.67	9/1123 (0.8%)
1	E	1.07	0/825	1.69	16/1114 (1.4%)
1	F	1.16	1/832 (0.1%)	1.71	12/1123 (1.1%)
1	G	1.13	0/829	1.72	12/1119 (1.1%)
1	H	1.16	0/829	1.68	11/1119 (1.0%)
All	All	1.13	2/6644 (0.0%)	1.70	94/8969 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	2	0
1	G	1	0
1	H	1	0
All	All	4	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	74	HIS	CA-C	-5.96	1.45	1.52
1	D	101	VAL	CA-CB	-5.67	1.48	1.54

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	HIS	CA-CB-CG	-10.22	103.58	113.80
1	F	47	PHE	CA-CB-CG	-8.37	105.43	113.80
1	G	95	PHE	CA-CB-CG	-8.16	105.64	113.80
1	C	6	HIS	CA-CB-CG	-8.16	105.64	113.80
1	B	80	HIS	N-CA-C	8.12	119.76	111.07
1	H	64	PRO	CB-CA-C	-7.89	99.08	110.75
1	D	75	ILE	N-CA-C	7.83	119.07	108.11
1	C	17	LEU	N-CA-C	7.79	123.38	113.25
1	D	101	VAL	N-CA-C	7.59	118.33	110.36
1	E	89	ASP	CA-CB-CG	-7.58	105.02	112.60
1	D	21	ARG	N-CA-CB	7.32	120.87	110.12
1	B	80	HIS	N-CA-CB	7.14	120.37	110.01
1	H	24	GLY	CA-C-N	-6.96	112.37	122.19
1	H	24	GLY	C-N-CA	-6.96	112.37	122.19
1	A	80	HIS	CA-CB-CG	-6.96	106.84	113.80
1	G	35	PHE	CA-CB-CG	-6.91	106.89	113.80
1	H	89	ASP	CA-CB-CG	-6.89	105.71	112.60
1	F	91	ASN	CA-CB-CG	-6.84	105.76	112.60
1	H	65	GLU	N-CA-C	-6.83	97.59	108.73
1	C	74	HIS	CA-CB-CG	-6.71	107.08	113.80
1	C	47	PHE	CA-CB-CG	-6.63	107.17	113.80
1	E	91	ASN	CA-CB-CG	-6.62	105.98	112.60
1	B	91	ASN	CA-CB-CG	-6.54	106.06	112.60
1	B	99	VAL	N-CA-C	6.51	116.67	110.42
1	E	29	GLU	N-CA-CB	6.37	119.70	110.20
1	E	37	GLN	CA-CB-CG	-6.36	101.38	114.10
1	G	66	TRP	N-CA-C	6.35	119.54	109.50
1	B	69	VAL	CB-CA-C	-6.34	101.50	110.12
1	A	73	VAL	CA-CB-CG2	6.30	121.11	110.40
1	D	89	ASP	CA-CB-CG	-6.18	106.42	112.60
1	B	24	GLY	CA-C-N	-6.16	111.26	120.94
1	B	24	GLY	C-N-CA	-6.16	111.26	120.94
1	F	60	LEU	CB-CA-C	-6.14	97.86	110.38
1	E	62	HIS	CA-CB-CG	-6.12	107.68	113.80
1	E	31	ARG	N-CA-C	6.11	116.15	108.45
1	G	66	TRP	CA-C-N	-6.00	113.00	122.73
1	G	66	TRP	C-N-CA	-6.00	113.00	122.73
1	D	48	GLY	N-CA-C	-5.92	105.63	112.73
1	H	42	ASP	N-CA-C	5.92	115.91	108.45
1	G	83	ALA	CB-CA-C	-5.89	98.69	110.42
1	C	22	ALA	CA-C-N	5.88	128.52	120.46
1	C	22	ALA	C-N-CA	5.88	128.52	120.46
1	F	99	VAL	O-C-N	-5.87	116.17	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	65	GLU	CA-C-N	-5.86	113.39	122.59
1	E	65	GLU	C-N-CA	-5.86	113.39	122.59
1	F	74	HIS	CA-CB-CG	-5.77	108.03	113.80
1	H	50	MET	CA-CB-CG	-5.77	102.57	114.10
1	E	21	ARG	N-CA-CB	-5.70	101.72	110.16
1	F	89	ASP	CA-CB-CG	-5.64	106.95	112.60
1	B	95	PHE	CA-CB-CG	-5.62	108.18	113.80
1	E	14	ASP	CA-CB-CG	5.61	118.20	112.60
1	B	40	PHE	CA-CB-CG	-5.53	108.27	113.80
1	H	31	ARG	N-CA-C	5.51	118.90	110.20
1	A	95	PHE	CA-CB-CG	-5.49	108.31	113.80
1	B	77	LEU	N-CA-C	5.49	117.35	108.34
1	A	80	HIS	CB-CA-C	5.49	119.59	110.81
1	D	67	PHE	CA-CB-CG	-5.49	108.31	113.80
1	E	35	PHE	CA-CB-CG	-5.48	108.32	113.80
1	E	17	LEU	N-CA-C	5.48	120.20	112.75
1	B	69	VAL	N-CA-CB	5.47	120.09	111.99
1	A	71	ASN	N-CA-C	5.45	119.63	112.92
1	A	74	HIS	CA-C-N	-5.45	115.55	123.06
1	A	74	HIS	C-N-CA	-5.45	115.55	123.06
1	E	19	ASN	N-CA-C	5.43	117.20	111.28
1	B	80	HIS	CA-CB-CG	-5.42	108.38	113.80
1	H	32	ASP	N-CA-CB	5.42	118.38	110.58
1	A	48	GLY	N-CA-C	-5.40	106.25	112.73
1	F	96	ILE	N-CA-CB	-5.38	104.53	110.51
1	D	36	LYS	CA-C-N	-5.38	115.13	122.93
1	D	36	LYS	C-N-CA	-5.38	115.13	122.93
1	F	19	ASN	CA-CB-CG	-5.36	107.24	112.60
1	E	20	LEU	CA-C-O	5.35	126.10	119.79
1	B	47	PHE	CA-CB-CG	-5.34	108.45	113.80
1	H	26	ASN	CA-CB-CG	-5.34	107.26	112.60
1	C	31	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	C	31	ARG	N-CA-C	5.27	117.08	109.07
1	A	98	GLN	CB-CA-C	-5.27	102.61	110.88
1	G	95	PHE	N-CA-C	-5.25	105.45	111.07
1	H	87	GLU	N-CA-CB	5.23	117.73	109.94
1	F	35	PHE	CA-CB-CG	5.22	119.02	113.80
1	E	15	GLN	CA-C-N	5.21	127.72	120.63
1	E	15	GLN	C-N-CA	5.21	127.72	120.63
1	F	8	LEU	O-C-N	5.18	129.28	123.06
1	D	7	ARG	N-CA-CB	5.16	119.20	110.49
1	G	11	GLU	N-CA-C	-5.16	104.59	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	9	SER	N-CA-C	-5.08	102.49	110.36
1	G	66	TRP	O-C-N	-5.07	117.00	123.24
1	F	75	ILE	N-CA-C	5.07	115.21	108.11
1	G	48	GLY	N-CA-C	-5.05	106.53	112.64
1	B	18	PRO	N-CA-CB	5.03	108.53	103.25
1	F	69	VAL	CB-CA-C	-5.01	103.65	110.42
1	C	82	CYS	N-CA-CB	5.01	117.89	110.53
1	G	97	GLU	CA-C-N	-5.01	113.93	120.44
1	G	97	GLU	C-N-CA	-5.01	113.93	120.44

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	6	HIS	CA
1	C	104	THR	CA
1	G	104	THR	CB
1	H	6	HIS	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	811	0	776	54	0
1	B	811	0	776	62	0
1	C	815	0	782	59	4
1	D	812	0	780	53	0
1	E	806	0	773	49	0
1	F	812	0	780	36	0
1	G	810	0	777	43	1
1	H	810	0	777	44	1
2	A	17	0	13	2	0
2	B	17	0	13	2	0
2	C	17	0	13	4	0
2	D	17	0	13	2	0
2	E	17	0	13	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	17	0	13	3	0
2	G	17	0	13	1	0
2	H	17	0	13	0	0
3	A	35	0	0	3	0
3	B	31	0	0	2	0
3	C	36	0	0	10	0
3	D	27	0	0	1	0
3	E	28	0	0	2	0
3	F	27	0	0	4	4
3	G	41	0	0	6	0
3	H	33	0	0	2	2
All	All	6881	0	6325	393	6

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 30.

All (393) 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:A:34:ILE:HG23	1:A:85:LEU:HD11	1.32	1.07
1:E:9:SER:HB3	1:E:12:GLU:HG3	1.41	1.03
1:H:19:ASN:H	1:H:19:ASN:HD22	1.20	0.90
1:H:91:ASN:N	1:H:91:ASN:HD22	1.63	0.89
1:C:37:GLN:HB2	1:C:74:HIS:CD2	2.09	0.87
1:E:9:SER:HB3	1:E:12:GLU:CG	2.05	0.85
1:H:91:ASN:H	1:H:91:ASN:ND2	1.78	0.81
1:B:67:PHE:CE1	1:B:69:VAL:HG22	2.15	0.81
1:F:52:ARG:HD2	1:H:44:ASN:OD1	1.81	0.80
1:B:58:GLU:HB3	3:C:125:HOH:O	1.82	0.80
1:D:7:ARG:O	1:D:8:LEU:C	2.27	0.78
1:F:6:HIS:ND1	1:F:82:CYS:HB3	1.98	0.77
1:C:56:GLN:HA	1:C:56:GLN:NE2	2.00	0.77
1:H:19:ASN:H	1:H:19:ASN:ND2	1.82	0.77
1:A:37:GLN:HB2	1:A:74:HIS:CD2	2.20	0.76
1:E:80:HIS:H	2:E:105:HBI:H3	1.32	0.76
1:F:45:ARG:HG2	1:F:103:MET:HG3	1.67	0.76
1:A:41:LYS:HG2	1:A:45:ARG:NH1	2.00	0.76
1:E:25:TRP:CE3	1:E:34:ILE:HG13	2.20	0.75
1:C:35:PHE:HB3	3:C:141:HOH:O	1.85	0.75
1:H:104:THR:HG22	3:H:134:HOH:O	1.87	0.75
1:H:91:ASN:N	1:H:91:ASN:ND2	2.28	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:CG2	1:A:85:LEU:HD11	2.14	0.74
1:G:9:SER:OG	1:G:12:GLU:HG3	1.88	0.74
1:F:35:PHE:HB3	3:F:125:HOH:O	1.87	0.73
1:G:92:LEU:O	1:G:96:ILE:HG13	1.87	0.73
1:A:39:HIS:HB2	3:A:113:HOH:O	1.86	0.73
1:D:28:LEU:HD23	1:D:31:ARG:HB2	1.70	0.73
1:E:46:ALA:O	1:E:49:PHE:HB3	1.87	0.73
1:B:44:ASN:ND2	1:D:55:LEU:HB2	2.04	0.72
1:A:87:GLU:O	1:A:90:ILE:HB	1.89	0.72
1:C:36:LYS:HE2	1:C:38:PHE:CZ	2.24	0.72
1:B:97:GLU:O	1:B:101:VAL:HG13	1.90	0.72
1:A:37:GLN:HB2	1:A:74:HIS:HD2	1.55	0.71
1:D:80:HIS:H	2:D:105:HBI:H3	1.35	0.71
1:G:7:ARG:HA	1:G:85:LEU:O	1.91	0.71
1:H:91:ASN:HD22	1:H:91:ASN:H	1.34	0.71
1:E:39:HIS:HB3	3:E:120:HOH:O	1.89	0.70
1:G:39:HIS:HB2	3:G:137:HOH:O	1.92	0.70
1:C:56:GLN:HA	1:C:56:GLN:HE21	1.55	0.70
1:C:11:GLU:HG3	3:C:119:HOH:O	1.92	0.70
1:D:9:SER:N	1:D:12:GLU:OE1	2.25	0.69
1:E:42:ASP:OD1	1:E:45:ARG:HB2	1.93	0.69
1:A:42:ASP:HB2	3:A:132:HOH:O	1.93	0.69
1:B:103:MET:O	1:B:104:THR:C	2.34	0.68
1:E:56:GLN:HG3	1:E:95:PHE:CZ	2.28	0.68
1:C:6:HIS:HA	3:C:116:HOH:O	1.94	0.68
1:C:8:LEU:O	1:C:13:ARG:NH1	2.27	0.67
1:C:13:ARG:NH2	1:C:32:ASP:OD2	2.27	0.67
1:D:36:LYS:HG3	1:D:37:GLN:N	2.07	0.67
1:H:92:LEU:O	1:H:96:ILE:HG13	1.95	0.67
1:D:12:GLU:O	1:D:13:ARG:C	2.36	0.66
1:B:61:ASP:O	2:B:105:HBI:H71	1.95	0.66
1:E:16:LEU:C	1:E:18:PRO:HD2	2.21	0.66
1:D:58:GLU:OE1	1:D:58:GLU:HA	1.96	0.66
1:H:11:GLU:O	1:H:15:GLN:HG3	1.95	0.66
1:A:46:ALA:O	1:A:49:PHE:HB3	1.95	0.66
1:G:9:SER:N	1:G:12:GLU:OE2	2.28	0.65
1:G:104:THR:HG23	3:G:139:HOH:O	1.95	0.65
1:F:56:GLN:NE2	3:F:110:HOH:O	2.29	0.65
1:H:79:THR:HB	1:H:82:CYS:SG	2.36	0.65
2:F:105:HBI:H113	3:F:130:HOH:O	1.97	0.64
1:A:17:LEU:N	1:A:18:PRO:HD2	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:NH2	1:B:65:GLU:OE2	2.29	0.64
1:C:9:SER:O	1:C:13:ARG:HG3	1.97	0.64
1:G:7:ARG:HD2	1:G:83:ALA:HB3	1.78	0.64
1:C:102:SER:N	3:C:124:HOH:O	2.29	0.63
1:E:35:PHE:HA	1:E:75:ILE:O	1.99	0.63
1:C:36:LYS:HE2	1:C:38:PHE:CE2	2.34	0.63
1:B:86:SER:OG	1:B:88:ARG:HB2	1.98	0.62
1:F:79:THR:HA	2:F:105:HBI:H3	1.63	0.62
1:B:21:ARG:HH11	1:B:21:ARG:CG	2.12	0.62
1:A:8:LEU:HG	1:A:86:SER:HA	1.80	0.62
1:B:8:LEU:HB3	1:B:13:ARG:HG2	1.82	0.62
1:D:9:SER:O	1:D:13:ARG:HG3	1.99	0.62
1:H:37:GLN:HB3	1:H:74:HIS:ND1	2.15	0.61
1:B:25:TRP:NE1	1:B:97:GLU:OE2	2.30	0.61
1:E:94:SER:O	1:E:97:GLU:HB2	1.99	0.61
1:B:12:GLU:O	1:B:16:LEU:HG	2.00	0.61
1:D:16:LEU:C	1:D:18:PRO:HD2	2.25	0.61
1:B:91:ASN:OD1	1:B:91:ASN:N	2.30	0.61
1:G:13:ARG:NH2	1:G:32:ASP:OD2	2.33	0.61
1:C:77:LEU:HA	3:C:133:HOH:O	2.01	0.60
1:A:43:PHE:HB2	1:A:70:TYR:CD1	2.36	0.60
1:A:63:HIS:ND1	2:A:105:HBI:N8	2.50	0.60
1:A:9:SER:O	1:A:13:ARG:HG3	2.02	0.60
1:H:37:GLN:HB3	1:H:74:HIS:CE1	2.36	0.60
1:B:37:GLN:NE2	1:B:38:PHE:O	2.34	0.60
1:H:102:SER:O	1:H:104:THR:HG23	2.02	0.60
1:F:67:PHE:CE2	1:F:69:VAL:HG23	2.36	0.60
1:E:56:GLN:HG3	1:E:95:PHE:CE2	2.37	0.59
1:B:58:GLU:HA	1:B:58:GLU:OE1	2.03	0.59
1:C:56:GLN:NE2	1:C:59:LYS:HB3	2.18	0.59
1:A:19:ASN:O	1:A:23:VAL:HG22	2.03	0.59
1:A:102:SER:O	1:A:103:MET:HG2	2.03	0.59
1:D:87:GLU:O	1:D:90:ILE:HB	2.02	0.59
1:D:97:GLU:O	1:D:100:ALA:HB3	2.02	0.59
1:D:12:GLU:HB3	1:D:16:LEU:HD11	1.85	0.59
1:D:46:ALA:O	1:D:50:MET:HG3	2.02	0.59
1:E:8:LEU:HB3	1:E:13:ARG:NH1	2.17	0.59
1:F:35:PHE:CE1	1:F:74:HIS:HB3	2.37	0.59
1:C:63:HIS:ND1	2:C:105:HBI:N8	2.51	0.58
1:D:9:SER:OG	1:D:10:ALA:N	2.30	0.58
1:B:21:ARG:HH11	1:B:21:ARG:CB	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:SER:O	1:E:12:GLU:HB2	2.03	0.58
1:H:19:ASN:ND2	1:H:19:ASN:N	2.50	0.58
1:G:13:ARG:HH22	1:G:32:ASP:CG	2.10	0.58
1:B:13:ARG:NH2	1:B:32:ASP:OD2	2.35	0.58
1:A:56:GLN:HG3	1:A:95:PHE:CZ	2.39	0.58
1:G:19:ASN:ND2	3:G:133:HOH:O	2.35	0.58
1:G:79:THR:HA	2:G:105:HBI:H3	1.69	0.58
1:B:37:GLN:HE21	1:B:38:PHE:N	2.02	0.57
1:C:8:LEU:HB2	1:C:13:ARG:NH1	2.18	0.57
1:B:67:PHE:HE1	1:B:69:VAL:HG22	1.63	0.57
1:E:69:VAL:HG13	1:F:65:GLU:HG2	1.86	0.57
1:G:28:LEU:HD12	1:G:33:ALA:HB3	1.85	0.57
1:B:16:LEU:C	1:B:18:PRO:HD2	2.30	0.57
1:H:87:GLU:O	1:H:91:ASN:ND2	2.37	0.57
1:E:56:GLN:HG3	1:E:95:PHE:CE1	2.39	0.57
1:A:65:GLU:HG3	1:B:69:VAL:HG13	1.88	0.56
1:D:40:PHE:O	1:D:71:ASN:ND2	2.28	0.56
1:B:37:GLN:O	1:B:37:GLN:HG3	2.03	0.56
1:B:67:PHE:HE1	1:B:69:VAL:CG2	2.18	0.56
1:F:95:PHE:O	1:F:99:VAL:HG23	2.05	0.56
1:C:35:PHE:CE1	1:C:74:HIS:HB3	2.41	0.56
1:C:42:ASP:OD1	1:C:45:ARG:HB2	2.05	0.56
1:C:93:ALA:HA	1:C:96:ILE:HD12	1.87	0.56
1:B:44:ASN:HD22	1:D:55:LEU:HB2	1.69	0.56
1:B:10:ALA:HA	1:B:13:ARG:HG3	1.88	0.56
1:D:10:ALA:O	1:D:13:ARG:N	2.39	0.56
1:F:92:LEU:O	1:F:96:ILE:HG13	2.05	0.56
1:D:36:LYS:HG2	1:D:38:PHE:CE1	2.41	0.55
1:A:31:ARG:NH2	1:A:65:GLU:OE1	2.40	0.55
1:C:16:LEU:N	1:C:16:LEU:HD23	2.20	0.55
1:A:32:ASP:HB3	1:A:84:GLY:HA2	1.88	0.54
1:D:82:CYS:O	1:D:83:ALA:C	2.49	0.54
1:G:39:HIS:N	3:G:138:HOH:O	2.38	0.54
1:C:62:HIS:NE2	2:C:105:HBI:N2	2.55	0.54
1:B:40:PHE:O	1:B:71:ASN:ND2	2.41	0.54
1:B:81:GLU:O	1:B:83:ALA:N	2.40	0.54
1:D:23:VAL:HG12	1:D:23:VAL:O	2.08	0.54
1:D:11:GLU:O	1:D:14:ASP:C	2.51	0.54
1:C:43:PHE:HB2	1:C:70:TYR:CD1	2.43	0.53
1:H:9:SER:H	1:H:12:GLU:CD	2.17	0.53
1:B:88:ARG:HA	1:B:91:ASN:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:GLN:HB2	1:C:74:HIS:HD2	1.65	0.53
1:D:33:ALA:HA	1:D:85:LEU:HD21	1.88	0.53
1:B:21:ARG:HH11	1:B:21:ARG:HG2	1.73	0.53
1:E:17:LEU:O	1:E:18:PRO:C	2.51	0.53
1:G:56:GLN:HA	1:G:56:GLN:OE1	2.07	0.53
1:B:94:SER:O	1:B:98:GLN:HG2	2.09	0.53
1:D:12:GLU:HB3	1:D:16:LEU:CD1	2.39	0.53
1:H:56:GLN:HG3	1:H:95:PHE:CG	2.43	0.53
1:D:11:GLU:O	1:D:15:GLN:HB2	2.08	0.53
1:F:35:PHE:CZ	1:F:74:HIS:HB3	2.43	0.53
1:G:23:VAL:HG22	1:G:23:VAL:O	2.08	0.52
1:E:39:HIS:CD2	1:E:72:LYS:HG2	2.44	0.52
1:G:95:PHE:O	1:G:96:ILE:C	2.48	0.52
1:E:11:GLU:O	1:E:12:GLU:C	2.51	0.52
1:H:56:GLN:HG2	1:H:95:PHE:CZ	2.45	0.52
1:D:17:LEU:N	1:D:18:PRO:CD	2.72	0.52
1:A:18:PRO:HD3	1:A:21:ARG:NH1	2.25	0.52
1:A:56:GLN:HG3	1:A:95:PHE:CE1	2.44	0.52
1:D:30:GLY:O	1:D:31:ARG:HG2	2.10	0.52
1:E:95:PHE:CE2	1:E:99:VAL:HG21	2.44	0.52
1:C:102:SER:HB3	3:C:124:HOH:O	2.09	0.51
1:G:35:PHE:CD2	1:G:74:HIS:CE1	2.98	0.51
1:A:102:SER:C	1:A:103:MET:HG2	2.35	0.51
1:H:67:PHE:CE2	1:H:69:VAL:HG23	2.45	0.51
1:C:33:ALA:HB2	1:C:78:SER:HB2	1.91	0.51
1:E:101:VAL:O	1:E:103:MET:N	2.42	0.51
1:G:44:ASN:ND2	3:G:111:HOH:O	2.39	0.51
1:C:13:ARG:NH2	3:C:140:HOH:O	2.34	0.51
1:C:62:HIS:CE1	1:C:88:ARG:HB2	2.45	0.51
1:F:9:SER:OG	1:F:12:GLU:HG3	2.10	0.51
1:F:51:THR:O	1:F:52:ARG:C	2.53	0.51
1:H:8:LEU:HA	1:H:12:GLU:OE1	2.11	0.51
1:H:86:SER:HB2	3:H:123:HOH:O	2.11	0.51
1:C:42:ASP:HB2	3:C:109:HOH:O	2.09	0.50
1:D:56:GLN:OE1	1:D:56:GLN:HA	2.10	0.50
1:F:42:ASP:OD1	1:F:45:ARG:HB2	2.11	0.50
1:C:62:HIS:CE1	2:C:105:HBI:N2	2.78	0.50
1:B:87:GLU:O	1:B:91:ASN:OD1	2.29	0.50
1:E:66:TRP:H	1:E:66:TRP:CD1	2.30	0.50
1:F:35:PHE:HZ	1:F:74:HIS:CD2	2.29	0.50
1:A:41:LYS:HG2	1:A:45:ARG:HH12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:PHE:CZ	1:H:69:VAL:CG2	2.95	0.50
1:A:26:ASN:O	1:A:34:ILE:HA	2.12	0.50
1:A:13:ARG:HB3	1:A:17:LEU:HD12	1.93	0.50
1:A:101:VAL:C	1:A:103:MET:H	2.19	0.50
1:B:79:THR:HB	1:B:82:CYS:SG	2.51	0.50
1:D:45:ARG:HG2	1:D:103:MET:HG2	1.94	0.50
1:F:57:ALA:O	1:F:61:ASP:N	2.45	0.50
1:G:34:ILE:HG23	1:G:85:LEU:HD11	1.93	0.50
1:F:35:PHE:HZ	1:F:74:HIS:HD2	1.59	0.50
1:G:17:LEU:HD12	1:G:21:ARG:HH21	1.76	0.49
1:H:62:HIS:CE1	1:H:88:ARG:HG3	2.47	0.49
1:H:95:PHE:O	1:H:96:ILE:C	2.54	0.49
1:A:32:ASP:O	1:A:78:SER:OG	2.30	0.49
1:E:63:HIS:ND1	2:E:105:HBI:N8	2.61	0.49
1:E:77:LEU:HD12	1:E:93:ALA:HB2	1.93	0.49
1:E:30:GLY:N	3:E:124:HOH:O	2.41	0.49
1:D:7:ARG:O	1:D:8:LEU:O	2.31	0.49
1:G:11:GLU:O	1:G:12:GLU:C	2.52	0.49
1:E:13:ARG:NH2	1:E:32:ASP:OD1	2.46	0.49
1:B:36:LYS:HE2	1:B:38:PHE:CE2	2.48	0.49
1:D:66:TRP:CD1	1:D:66:TRP:N	2.79	0.49
1:G:17:LEU:N	1:G:18:PRO:CD	2.75	0.48
1:E:66:TRP:CD1	1:E:66:TRP:N	2.79	0.48
1:H:34:ILE:O	1:H:76:THR:HA	2.12	0.48
1:B:9:SER:OG	1:B:12:GLU:OE1	2.28	0.48
1:D:57:ALA:HB1	1:D:62:HIS:O	2.12	0.48
1:F:26:ASN:O	1:F:34:ILE:HA	2.13	0.48
1:B:21:ARG:HG2	1:B:21:ARG:NH1	2.28	0.48
1:C:60:LEU:C	1:C:60:LEU:HD12	2.38	0.48
1:D:45:ARG:HG2	1:D:103:MET:HB3	1.95	0.48
1:E:77:LEU:CD1	1:E:93:ALA:HB2	2.44	0.48
1:H:43:PHE:O	1:H:44:ASN:C	2.53	0.48
1:H:56:GLN:HG3	1:H:95:PHE:CD2	2.49	0.48
1:A:88:ARG:O	1:A:89:ASP:C	2.56	0.48
1:C:9:SER:N	1:C:12:GLU:OE1	2.43	0.48
1:H:13:ARG:O	1:H:18:PRO:HD3	2.13	0.48
1:E:34:ILE:O	1:E:77:LEU:N	2.41	0.48
1:F:70:TYR:HD2	1:F:71:ASN:OD1	1.96	0.48
1:A:37:GLN:O	1:A:37:GLN:HG3	2.14	0.48
1:F:63:HIS:ND1	2:F:105:HBI:N8	2.57	0.48
1:F:7:ARG:HA	1:F:85:LEU:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH2	1:A:76:THR:HG21	2.29	0.47
1:A:32:ASP:CG	1:A:85:LEU:H	2.21	0.47
1:F:17:LEU:N	1:F:18:PRO:CD	2.77	0.47
1:B:81:GLU:O	1:B:82:CYS:C	2.57	0.47
1:D:17:LEU:N	1:D:18:PRO:HD2	2.28	0.47
1:C:53:VAL:HG22	1:C:66:TRP:CH2	2.49	0.47
1:E:90:ILE:H	1:E:90:ILE:HG12	1.48	0.47
1:C:67:PHE:HD2	1:C:74:HIS:ND1	2.13	0.47
1:H:13:ARG:O	1:H:17:LEU:HB2	2.15	0.47
1:E:25:TRP:CE3	1:E:36:LYS:HB2	2.49	0.47
1:A:6:HIS:O	1:A:8:LEU:N	2.48	0.47
1:B:60:LEU:O	1:B:61:ASP:HB3	2.14	0.47
1:E:62:HIS:CD2	1:E:88:ARG:HB3	2.49	0.47
1:G:7:ARG:HH11	1:G:83:ALA:CB	2.28	0.47
1:H:17:LEU:N	1:H:18:PRO:CD	2.77	0.47
1:A:9:SER:HB3	1:A:12:GLU:OE1	2.14	0.47
1:F:67:PHE:CE2	1:F:69:VAL:CG2	2.97	0.47
1:A:17:LEU:HB2	1:A:21:ARG:NH2	2.30	0.47
1:B:67:PHE:CZ	1:B:69:VAL:HG22	2.49	0.47
1:D:10:ALA:O	1:D:12:GLU:N	2.48	0.47
1:F:17:LEU:N	1:F:18:PRO:HD2	2.30	0.47
1:G:69:VAL:HG13	1:H:65:GLU:HG2	1.97	0.47
1:A:17:LEU:N	1:A:18:PRO:CD	2.78	0.46
1:A:87:GLU:HB2	3:A:128:HOH:O	2.14	0.46
1:B:66:TRP:CD1	1:B:66:TRP:N	2.82	0.46
1:E:17:LEU:N	1:E:18:PRO:CD	2.78	0.46
1:H:86:SER:O	1:H:87:GLU:C	2.58	0.46
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.60	0.46
1:D:86:SER:OG	1:D:88:ARG:HB2	2.15	0.46
1:G:26:ASN:O	1:G:34:ILE:HA	2.16	0.46
1:D:63:HIS:ND1	2:D:105:HBI:N8	2.63	0.46
1:D:66:TRP:CD1	1:D:66:TRP:H	2.34	0.46
1:G:17:LEU:O	1:G:18:PRO:C	2.59	0.46
1:E:56:GLN:CG	1:E:95:PHE:CZ	2.98	0.46
1:F:9:SER:O	1:F:10:ALA:C	2.57	0.46
1:G:85:LEU:HD22	1:G:89:ASP:HB2	1.97	0.46
1:C:62:HIS:CE1	1:C:88:ARG:CB	2.99	0.46
1:G:20:LEU:HD23	1:G:20:LEU:HA	1.74	0.46
1:E:15:GLN:HE22	1:E:16:LEU:HD23	1.81	0.46
1:G:80:HIS:O	1:G:81:GLU:C	2.60	0.46
1:G:82:CYS:O	1:G:83:ALA:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:PHE:CE2	1:C:69:VAL:HG23	2.52	0.45
1:D:52:ARG:HA	1:D:55:LEU:HD12	1.99	0.45
1:F:67:PHE:CZ	1:F:69:VAL:CG2	2.99	0.45
1:B:25:TRP:CZ3	1:B:34:ILE:HD12	2.51	0.45
1:C:63:HIS:HA	1:C:64:PRO:HD3	1.79	0.45
1:D:67:PHE:CE2	1:D:69:VAL:CG2	2.99	0.45
1:D:12:GLU:H	1:D:12:GLU:HG3	1.61	0.45
1:E:25:TRP:CD2	1:E:36:LYS:HB2	2.51	0.45
1:A:36:LYS:CG	1:A:37:GLN:N	2.80	0.45
1:B:91:ASN:O	1:B:92:LEU:C	2.57	0.45
1:A:97:GLU:HA	1:A:97:GLU:OE1	2.17	0.45
1:D:37:GLN:HG3	1:D:38:PHE:N	2.31	0.45
1:H:95:PHE:CE2	1:H:99:VAL:HG21	2.52	0.45
1:B:25:TRP:CE3	1:B:34:ILE:CD1	3.00	0.45
1:F:92:LEU:HD12	1:F:92:LEU:HA	1.60	0.45
1:G:35:PHE:CD2	1:G:74:HIS:NE2	2.84	0.45
1:B:21:ARG:HA	1:B:25:TRP:O	2.16	0.45
1:D:35:PHE:HA	1:D:75:ILE:O	2.16	0.45
1:F:42:ASP:HB2	3:F:111:HOH:O	2.16	0.45
1:E:17:LEU:N	1:E:18:PRO:HD2	2.31	0.45
1:G:90:ILE:O	1:G:93:ALA:HB3	2.17	0.45
1:C:67:PHE:CZ	1:C:69:VAL:CG2	2.99	0.44
1:G:93:ALA:O	1:G:96:ILE:HB	2.16	0.44
1:A:80:HIS:H	2:A:105:HBI:H3	1.64	0.44
1:B:46:ALA:O	1:B:50:MET:HG3	2.17	0.44
1:C:40:PHE:O	1:C:71:ASN:ND2	2.49	0.44
1:E:87:GLU:O	1:E:91:ASN:HB2	2.16	0.44
1:A:95:PHE:CE2	1:A:99:VAL:HG21	2.53	0.44
1:B:45:ARG:NE	3:B:113:HOH:O	2.28	0.44
1:B:80:HIS:H	2:B:105:HBI:H3	1.66	0.44
1:C:56:GLN:HE21	1:C:56:GLN:CA	2.25	0.44
1:A:16:LEU:C	1:A:18:PRO:HD2	2.41	0.44
1:B:10:ALA:O	1:B:14:ASP:HB2	2.18	0.44
1:F:6:HIS:CE1	1:F:82:CYS:HB3	2.51	0.44
1:A:20:LEU:HA	1:A:20:LEU:HD23	1.75	0.43
1:C:97:GLU:O	1:C:101:VAL:HG23	2.18	0.43
1:D:25:TRP:CE3	1:D:34:ILE:HD12	2.53	0.43
1:H:67:PHE:CE2	1:H:69:VAL:CG2	3.02	0.43
1:G:75:ILE:HG21	1:G:75:ILE:HD13	1.66	0.43
1:A:35:PHE:CG	1:A:36:LYS:N	2.86	0.43
1:B:25:TRP:CE3	1:B:34:ILE:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ASN:O	1:C:92:LEU:C	2.57	0.43
1:G:26:ASN:HB2	1:G:35:PHE:CE1	2.53	0.43
1:G:32:ASP:HB3	1:G:84:GLY:HA3	2.00	0.43
1:C:43:PHE:HB2	1:C:70:TYR:CE1	2.54	0.43
1:C:66:TRP:CD1	1:C:66:TRP:N	2.85	0.43
1:H:69:VAL:O	1:H:70:TYR:C	2.59	0.43
1:C:28:LEU:HD21	1:C:35:PHE:HB2	2.00	0.43
1:B:69:VAL:O	1:B:70:TYR:C	2.61	0.43
1:C:95:PHE:CE1	1:C:99:VAL:HG21	2.53	0.43
1:H:87:GLU:O	1:H:90:ILE:N	2.52	0.43
1:A:66:TRP:HA	1:A:74:HIS:O	2.19	0.43
1:A:77:LEU:HD22	1:A:92:LEU:HD23	2.01	0.43
1:E:103:MET:HE2	1:G:52:ARG:HH11	1.83	0.43
1:B:42:ASP:OD1	1:B:45:ARG:HB2	2.19	0.42
1:G:9:SER:H	1:G:12:GLU:CD	2.27	0.42
1:G:90:ILE:HD13	1:G:90:ILE:HA	1.82	0.42
1:E:8:LEU:HB3	1:E:13:ARG:HH11	1.81	0.42
1:B:103:MET:H	1:B:103:MET:HG2	1.63	0.42
1:C:15:GLN:C	1:C:16:LEU:HD23	2.44	0.42
1:D:42:ASP:N	1:D:42:ASP:OD1	2.52	0.42
1:D:69:VAL:O	1:D:70:TYR:C	2.60	0.42
1:E:72:LYS:HB2	1:E:72:LYS:HE2	1.52	0.42
1:B:103:MET:O	1:B:104:THR:O	2.37	0.42
1:G:28:LEU:HD13	1:G:31:ARG:HD3	2.01	0.42
1:H:9:SER:HB3	1:H:12:GLU:OE2	2.20	0.42
1:B:86:SER:C	1:B:88:ARG:N	2.77	0.42
1:B:103:MET:HB2	1:B:104:THR:H	1.70	0.42
1:C:63:HIS:N	2:C:105:HBI:N1	2.62	0.42
1:F:6:HIS:HD1	1:F:82:CYS:HB3	1.79	0.42
1:H:45:ARG:HH11	1:H:104:THR:C	2.27	0.42
1:H:54:ALA:O	1:H:57:ALA:HB3	2.19	0.42
1:F:9:SER:O	1:F:12:GLU:N	2.37	0.42
1:E:18:PRO:O	1:E:21:ARG:HB3	2.20	0.42
1:C:12:GLU:O	1:C:16:LEU:HG	2.20	0.42
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.80	0.41
1:B:21:ARG:NH1	3:B:125:HOH:O	2.35	0.41
1:E:25:TRP:HE3	1:E:34:ILE:HG13	1.78	0.41
1:F:12:GLU:O	1:F:13:ARG:C	2.62	0.41
1:H:31:ARG:NH2	1:H:65:GLU:OE2	2.35	0.41
1:A:43:PHE:HB2	1:A:70:TYR:CE1	2.55	0.41
1:B:49:PHE:HB2	1:B:103:MET:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:ASN:HB2	1:E:35:PHE:CZ	2.54	0.41
1:E:36:LYS:NZ	1:E:97:GLU:OE2	2.53	0.41
1:B:35:PHE:HA	1:B:75:ILE:O	2.19	0.41
1:D:16:LEU:O	1:D:19:ASN:ND2	2.52	0.41
1:E:25:TRP:CE3	1:E:34:ILE:CG1	2.99	0.41
1:F:7:ARG:HH11	1:F:7:ARG:HD3	1.73	0.41
1:F:23:VAL:HG22	1:F:23:VAL:O	2.19	0.41
1:H:87:GLU:H	1:H:87:GLU:HG3	1.67	0.41
1:B:55:LEU:HD22	1:C:58:GLU:HG3	2.02	0.41
1:C:43:PHE:O	1:C:44:ASN:C	2.62	0.41
1:C:92:LEU:HA	1:C:92:LEU:HD12	1.72	0.41
1:C:8:LEU:C	1:C:13:ARG:NH1	2.78	0.41
1:C:85:LEU:HD22	3:C:140:HOH:O	2.20	0.41
1:D:99:VAL:O	1:D:100:ALA:C	2.63	0.41
1:A:17:LEU:HB2	1:A:21:ARG:CZ	2.50	0.41
1:A:101:VAL:C	1:A:103:MET:N	2.79	0.41
1:D:12:GLU:O	1:D:15:GLN:N	2.54	0.41
1:G:36:LYS:HA	3:G:129:HOH:O	2.21	0.41
1:B:95:PHE:CE2	1:B:99:VAL:HG21	2.56	0.41
1:D:17:LEU:O	1:D:20:LEU:N	2.53	0.41
1:G:28:LEU:HD23	1:G:28:LEU:HA	1.86	0.41
1:C:23:VAL:HG11	1:C:97:GLU:CD	2.46	0.41
1:F:74:HIS:ND1	1:F:74:HIS:N	2.69	0.41
1:C:35:PHE:CZ	1:C:74:HIS:HB3	2.55	0.41
1:C:79:THR:HB	1:C:86:SER:HB3	2.03	0.41
1:H:88:ARG:O	1:H:89:ASP:C	2.63	0.41
1:A:66:TRP:CD1	1:A:66:TRP:H	2.40	0.40
1:E:26:ASN:O	1:E:34:ILE:HA	2.21	0.40
1:B:36:LYS:HE2	1:B:38:PHE:CZ	2.56	0.40
1:B:88:ARG:O	1:B:91:ASN:OD1	2.39	0.40
1:C:80:HIS:ND1	1:C:80:HIS:C	2.78	0.40
1:E:13:ARG:NH2	1:E:32:ASP:CG	2.79	0.40
1:D:32:ASP:HA	3:D:117:HOH:O	2.20	0.40
1:D:32:ASP:OD2	1:D:85:LEU:N	2.48	0.40
1:A:95:PHE:CE2	1:A:99:VAL:CG2	3.05	0.40
1:B:85:LEU:HA	1:B:85:LEU:HD23	1.83	0.40
1:C:79:THR:OG1	1:C:89:ASP:OD2	2.28	0.40
1:D:93:ALA:O	1:D:96:ILE:HB	2.22	0.40
1:G:89:ASP:O	1:G:90:ILE:C	2.64	0.40
1:A:7:ARG:O	1:A:8:LEU:C	2.64	0.40
1:C:25:TRP:CD2	1:C:36:LYS:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:LEU:O	1:E:23:VAL:HG23	2.22	0.40
1:H:45:ARG:HG2	1:H:103:MET:HG2	2.04	0.40

All (6) 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:C:29:GLU:CD	3:F:124:HOH:O[2_664]	0.44	1.76
1:C:29:GLU:OE2	3:F:124:HOH:O[2_664]	0.86	1.34
1:C:29:GLU:OE1	3:F:124:HOH:O[2_664]	1.50	0.70
1:C:29:GLU:CG	3:F:124:HOH:O[2_664]	1.83	0.37
1:H:68:ASN:O	3:H:138:HOH:O[4_556]	2.11	0.09
1:G:66:TRP:O	3:H:138:HOH:O[4_556]	2.14	0.06

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	97/104 (93%)	88 (91%)	5 (5%)	4 (4%)	2	1
1	B	97/104 (93%)	90 (93%)	4 (4%)	3 (3%)	3	2
1	C	97/104 (93%)	93 (96%)	3 (3%)	1 (1%)	12	15
1	D	97/104 (93%)	84 (87%)	8 (8%)	5 (5%)	1	1
1	E	97/104 (93%)	85 (88%)	10 (10%)	2 (2%)	5	4
1	F	97/104 (93%)	90 (93%)	7 (7%)	0	100	100
1	G	97/104 (93%)	91 (94%)	5 (5%)	1 (1%)	12	15
1	H	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
All	All	776/832 (93%)	714 (92%)	46 (6%)	16 (2%)	5	4

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	LEU
1	D	9	SER
1	D	11	GLU
1	B	82	CYS
1	G	83	ALA
1	B	81	GLU
1	D	7	ARG
1	E	14	ASP
1	E	103	MET
1	A	102	SER
1	D	8	LEU
1	B	103	MET
1	A	18	PRO
1	D	90	ILE
1	C	64	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/88 (97%)	70 (82%)	15 (18%)	2	2
1	B	85/88 (97%)	70 (82%)	15 (18%)	2	2
1	C	86/88 (98%)	67 (78%)	19 (22%)	1	1
1	D	85/88 (97%)	73 (86%)	12 (14%)	3	3
1	E	84/88 (96%)	71 (84%)	13 (16%)	2	3
1	F	85/88 (97%)	73 (86%)	12 (14%)	3	3
1	G	85/88 (97%)	79 (93%)	6 (7%)	13	19
1	H	85/88 (97%)	71 (84%)	14 (16%)	2	2
All	All	680/704 (97%)	574 (84%)	106 (16%)	2	3

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	37	GLN
1	A	38	PHE
1	A	41	LYS
1	A	65	GLU
1	A	66	TRP
1	A	69	VAL
1	A	72	LYS
1	A	73	VAL
1	A	77	LEU
1	A	78	SER
1	A	81	GLU
1	A	87	GLU
1	A	102	SER
1	A	103	MET
1	B	8	LEU
1	B	11	GLU
1	B	21	ARG
1	B	29	GLU
1	B	34	ILE
1	B	37	GLN
1	B	41	LYS
1	B	58	GLU
1	B	68	ASN
1	B	69	VAL
1	B	91	ASN
1	B	98	GLN
1	B	101	VAL
1	B	103	MET
1	B	104	THR
1	C	6	HIS
1	C	21	ARG
1	C	26	ASN
1	C	28	LEU
1	C	37	GLN
1	C	41	LYS
1	C	45	ARG
1	C	49	PHE
1	C	53	VAL
1	C	56	GLN
1	C	69	VAL
1	C	72	LYS
1	C	81	GLU

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Mol	Chain	Res	Type
1	C	82	CYS
1	C	85	LEU
1	C	94	SER
1	C	98	GLN
1	C	103	MET
1	C	104	THR
1	D	12	GLU
1	D	19	ASN
1	D	36	LYS
1	D	45	ARG
1	D	58	GLU
1	D	66	TRP
1	D	72	LYS
1	D	82	CYS
1	D	91	ASN
1	D	94	SER
1	D	97	GLU
1	D	103	MET
1	E	19	ASN
1	E	31	ARG
1	E	34	ILE
1	E	36	LYS
1	E	41	LYS
1	E	45	ARG
1	E	59	LYS
1	E	66	TRP
1	E	72	LYS
1	E	86	SER
1	E	91	ASN
1	E	94	SER
1	E	103	MET
1	F	11	GLU
1	F	29	GLU
1	F	45	ARG
1	F	56	GLN
1	F	59	LYS
1	F	66	TRP
1	F	68	ASN
1	F	88	ARG
1	F	91	ASN
1	F	94	SER
1	F	102	SER

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Mol	Chain	Res	Type
1	F	104	THR
1	G	15	GLN
1	G	66	TRP
1	G	69	VAL
1	G	101	VAL
1	G	103	MET
1	G	104	THR
1	H	17	LEU
1	H	19	ASN
1	H	37	GLN
1	H	45	ARG
1	H	50	MET
1	H	56	GLN
1	H	68	ASN
1	H	69	VAL
1	H	73	VAL
1	H	87	GLU
1	H	88	ARG
1	H	91	ASN
1	H	102	SER
1	H	103	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	74	HIS
1	B	37	GLN
1	B	56	GLN
1	C	56	GLN
1	D	6	HIS
1	D	15	GLN
1	D	37	GLN
1	D	39	HIS
1	E	15	GLN
1	E	39	HIS
1	F	37	GLN
1	F	56	GLN
1	F	74	HIS
1	G	39	HIS
1	G	74	HIS
1	H	19	ASN

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Mol	Chain	Res	Type
1	H	56	GLN
1	H	91	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	HBI	F	105	-	15,18,18	3.06	7 (46%)	14,26,26	2.12	7 (50%)
2	HBI	D	105	-	15,18,18	3.16	9 (60%)	14,26,26	2.69	7 (50%)
2	HBI	B	105	-	15,18,18	3.20	6 (40%)	14,26,26	2.32	6 (42%)
2	HBI	E	105	-	15,18,18	3.28	8 (53%)	14,26,26	1.97	6 (42%)
2	HBI	H	105	-	15,18,18	3.21	8 (53%)	14,26,26	2.44	8 (57%)
2	HBI	A	105	-	15,18,18	3.46	8 (53%)	14,26,26	2.03	6 (42%)
2	HBI	C	105	-	15,18,18	3.23	8 (53%)	14,26,26	1.96	6 (42%)
2	HBI	G	105	-	15,18,18	3.33	7 (46%)	14,26,26	2.40	7 (50%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HBI	F	105	-	-	0/4/17/17	0/2/2/2
2	HBI	D	105	-	-	0/4/17/17	0/2/2/2
2	HBI	B	105	-	-	0/4/17/17	0/2/2/2
2	HBI	E	105	-	-	0/4/17/17	0/2/2/2
2	HBI	H	105	-	-	1/4/17/17	0/2/2/2
2	HBI	A	105	-	-	0/4/17/17	0/2/2/2
2	HBI	C	105	-	-	0/4/17/17	0/2/2/2
2	HBI	G	105	-	-	0/4/17/17	0/2/2/2

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	105	HBI	O4-C4	8.48	1.39	1.23
2	C	105	HBI	O4-C4	8.08	1.38	1.23
2	F	105	HBI	O4-C4	7.62	1.38	1.23
2	G	105	HBI	O4-C4	7.45	1.37	1.23
2	E	105	HBI	O4-C4	7.44	1.37	1.23
2	A	105	HBI	O4-C4	7.24	1.37	1.23
2	H	105	HBI	O4-C4	7.12	1.37	1.23
2	A	105	HBI	C7-C6	7.06	1.57	1.49
2	G	105	HBI	C7-C6	7.03	1.57	1.49
2	D	105	HBI	C7-C6	6.64	1.57	1.49
2	D	105	HBI	O4-C4	6.61	1.36	1.23
2	H	105	HBI	C7-C6	6.25	1.57	1.49
2	E	105	HBI	C7-C6	6.10	1.56	1.49
2	F	105	HBI	C7-C6	5.69	1.56	1.49
2	C	105	HBI	C7-C6	5.68	1.56	1.49
2	B	105	HBI	C7-C6	5.64	1.56	1.49
2	A	105	HBI	C7-N8	5.00	1.53	1.45
2	E	105	HBI	C7-N8	4.90	1.53	1.45
2	H	105	HBI	C7-N8	4.58	1.52	1.45
2	G	105	HBI	C7-N8	4.41	1.52	1.45
2	C	105	HBI	C7-N8	4.31	1.52	1.45
2	B	105	HBI	C7-N8	3.92	1.51	1.45
2	F	105	HBI	C7-N8	3.53	1.50	1.45
2	D	105	HBI	C11-C10	3.52	1.61	1.51
2	H	105	HBI	C4A-N5	3.30	1.44	1.37
2	D	105	HBI	C4A-N5	3.26	1.44	1.37
2	G	105	HBI	C4A-N5	3.12	1.44	1.37
2	A	105	HBI	C4-N3	-3.12	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	105	HBI	C2-N2	3.09	1.41	1.34
2	E	105	HBI	C4-N3	-3.07	1.33	1.38
2	H	105	HBI	C4-N3	-3.05	1.33	1.38
2	B	105	HBI	C4A-N5	3.04	1.44	1.37
2	F	105	HBI	C4A-N5	3.03	1.44	1.37
2	C	105	HBI	C4A-N5	3.03	1.44	1.37
2	E	105	HBI	C4A-N5	3.00	1.44	1.37
2	A	105	HBI	C4A-N5	2.91	1.43	1.37
2	F	105	HBI	C4-N3	-2.87	1.33	1.38
2	D	105	HBI	C4-N3	-2.83	1.33	1.38
2	D	105	HBI	C7-N8	2.82	1.49	1.45
2	G	105	HBI	C2-N2	2.79	1.40	1.34
2	C	105	HBI	C2-N2	2.63	1.40	1.34
2	E	105	HBI	C4A-C8A	2.52	1.46	1.40
2	B	105	HBI	C4-N3	-2.51	1.34	1.38
2	G	105	HBI	C4A-C8A	2.49	1.46	1.40
2	E	105	HBI	C2-N2	2.48	1.40	1.34
2	G	105	HBI	C4-N3	-2.47	1.34	1.38
2	B	105	HBI	C2-N2	2.46	1.39	1.34
2	F	105	HBI	C2-N3	-2.45	1.31	1.37
2	C	105	HBI	O9-C9	2.41	1.46	1.42
2	H	105	HBI	C4A-C8A	2.41	1.46	1.40
2	C	105	HBI	C4A-C8A	2.37	1.46	1.40
2	H	105	HBI	O9-C9	2.35	1.46	1.42
2	A	105	HBI	O9-C9	2.33	1.46	1.42
2	C	105	HBI	C4-N3	-2.31	1.34	1.38
2	D	105	HBI	C4A-C8A	2.29	1.45	1.40
2	A	105	HBI	C4A-C8A	2.24	1.45	1.40
2	E	105	HBI	C8A-N1	-2.20	1.32	1.36
2	F	105	HBI	C2-N2	2.19	1.39	1.34
2	D	105	HBI	C8A-N1	-2.14	1.32	1.36
2	H	105	HBI	C2-N2	2.03	1.38	1.34
2	D	105	HBI	C2-N2	2.00	1.38	1.34

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	105	HBI	O10-C10-C11	6.20	128.22	109.68
2	G	105	HBI	C2-N3-C4	-4.26	117.38	125.11
2	F	105	HBI	C2-N3-C4	-4.25	117.40	125.11
2	D	105	HBI	C2-N3-C4	-4.25	117.40	125.11
2	B	105	HBI	C2-N3-C4	-4.10	117.67	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	HBI	O4-C4-C4A	-4.02	115.92	126.53
2	G	105	HBI	O10-C10-C11	3.79	121.03	109.68
2	A	105	HBI	C2-N3-C4	-3.77	118.28	125.11
2	H	105	HBI	O10-C10-C11	3.71	120.77	109.68
2	E	105	HBI	C2-N3-C4	-3.68	118.44	125.11
2	C	105	HBI	C2-N3-C4	-3.64	118.50	125.11
2	H	105	HBI	C2-N3-C4	-3.59	118.60	125.11
2	H	105	HBI	C4A-N5-C6	3.41	123.40	116.08
2	H	105	HBI	N2-C2-N1	-3.41	113.02	119.67
2	F	105	HBI	C4A-N5-C6	3.28	123.11	116.08
2	G	105	HBI	C4A-C4-N3	3.17	121.32	113.25
2	B	105	HBI	O9-C9-C6	3.16	115.40	109.00
2	F	105	HBI	C4A-C4-N3	3.11	121.17	113.25
2	E	105	HBI	N2-C2-N1	-3.10	113.62	119.67
2	D	105	HBI	C4A-C4-N3	3.07	121.08	113.25
2	B	105	HBI	C4A-C4-N3	3.06	121.05	113.25
2	C	105	HBI	C4A-C4-N3	3.01	120.91	113.25
2	G	105	HBI	C4A-N5-C6	2.98	122.46	116.08
2	D	105	HBI	C4A-N5-C6	2.96	122.44	116.08
2	A	105	HBI	C4A-C4-N3	2.93	120.72	113.25
2	A	105	HBI	C4A-N5-C6	2.93	122.36	116.08
2	D	105	HBI	N2-C2-N1	-2.82	114.17	119.67
2	B	105	HBI	C4A-N5-C6	2.79	122.07	116.08
2	H	105	HBI	O4-C4-N3	-2.78	114.89	120.11
2	G	105	HBI	O4-C4-C4A	-2.75	119.27	126.53
2	E	105	HBI	C4A-N5-C6	2.75	121.98	116.08
2	C	105	HBI	C4A-N5-C6	2.69	121.85	116.08
2	E	105	HBI	N3-C2-N1	2.68	128.22	123.32
2	A	105	HBI	O4-C4-C4A	-2.59	119.71	126.53
2	A	105	HBI	N2-C2-N1	-2.57	114.66	119.67
2	C	105	HBI	N2-C2-N1	-2.56	114.67	119.67
2	E	105	HBI	C4A-C4-N3	2.55	119.75	113.25
2	H	105	HBI	C4A-C4-N3	2.51	119.65	113.25
2	E	105	HBI	O4-C4-C4A	-2.42	120.14	126.53
2	F	105	HBI	N3-C2-N1	2.41	127.74	123.32
2	G	105	HBI	N3-C2-N1	2.41	127.73	123.32
2	D	105	HBI	C2-N1-C8A	2.41	117.61	113.36
2	F	105	HBI	C2-N1-C8A	2.39	117.57	113.36
2	B	105	HBI	C2-N1-C8A	2.37	117.55	113.36
2	F	105	HBI	O4-C4-C4A	-2.36	120.31	126.53
2	H	105	HBI	O9-C9-C6	2.28	113.63	109.00
2	A	105	HBI	C2-N1-C8A	2.27	117.37	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	105	HBI	C2-N1-C8A	2.21	117.27	113.36
2	D	105	HBI	N3-C2-N1	2.21	127.37	123.32
2	H	105	HBI	N3-C2-N1	2.18	127.31	123.32
2	G	105	HBI	C2-N1-C8A	2.15	117.15	113.36
2	F	105	HBI	N2-C2-N1	-2.14	115.49	119.67
2	C	105	HBI	O4-C4-C4A	-2.14	120.89	126.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	105	HBI	C11-C10-C9-O9

There are no ring outliers.

7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	105	HBI	3	0
2	D	105	HBI	2	0
2	B	105	HBI	2	0
2	E	105	HBI	2	0
2	A	105	HBI	2	0
2	C	105	HBI	4	0
2	G	105	HBI	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

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.