



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:27 PM UTC

PDB ID : 3MON / pdb_00003mon
Title : CRYSTAL STRUCTURES OF TWO INTENSELY SWEET PROTEINS
Authors : Jiang, F.; Tong, L.; Kim, S.-H.
Deposited on : 1992-08-26
Resolution : 2.80 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

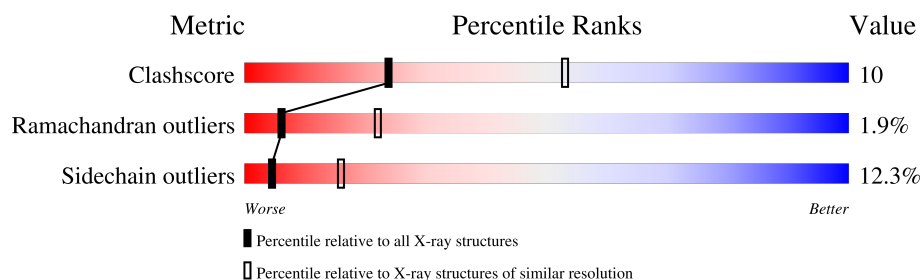
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	44	52% 39% 5% 5%
1	C	44	57% 36% 5% .
1	E	44	55% 36% 7% .
1	G	44	57% 32% 9% .
2	B	50	44% 30% 24% .
2	D	50	58% 26% 16%
2	F	50	60% 32% 6% .
2	H	50	56% 30% 10% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3136 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 MONELLIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	44	Total	C	N	O	0	0	0
			373	241	65	67			
1	C	44	Total	C	N	O	0	0	0
			373	241	65	67			
1	E	44	Total	C	N	O	0	0	0
			373	241	65	67			
1	G	44	Total	C	N	O	0	0	0
			373	241	65	67			

- Molecule 2 is a protein called MONELLIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	50	Total	C	N	O	S	0	0	0
			411	263	68	78	2			
2	D	50	Total	C	N	O	S	0	0	0
			411	263	68	78	2			
2	F	50	Total	C	N	O	S	0	0	0
			411	263	68	78	2			
2	H	50	Total	C	N	O	S	0	0	0
			411	263	68	78	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP P02882
D	?	-	GLU	deletion	UNP P02882
F	?	-	GLU	deletion	UNP P02882
H	?	-	GLU	deletion	UNP P02882

3 Residue-property plots [i](#)

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

Chain A: 



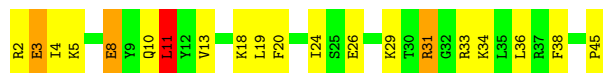
• Molecule 1: MONELLIN

Chain C: 



• Molecule 1: MONELLIN

Chain E: 



• Molecule 1: MONELLIN

Chain G: 



• Molecule 2: MONELLIN

Chain B: 

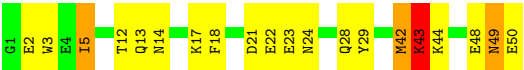


• Molecule 2: MONELLIN

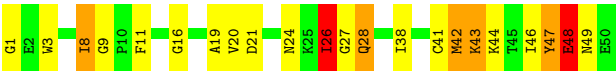
Chain D: 



• Molecule 2: MONELLIN



• Molecule 2: MONELLIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 1 21	Depositor
Cell constants a, b, c, α , β , γ	39.84Å 87.20Å 72.06Å 90.00° 90.00° 107.30°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.193 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3136	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.24	2/383 (0.5%)	2.01	12/514 (2.3%)
1	C	1.07	1/383 (0.3%)	1.91	12/514 (2.3%)
1	E	1.07	0/383	2.01	15/514 (2.9%)
1	G	1.12	1/383 (0.3%)	2.20	19/514 (3.7%)
2	B	1.18	2/419 (0.5%)	2.20	20/561 (3.6%)
2	D	1.01	0/419	1.95	11/561 (2.0%)
2	F	1.06	0/419	2.08	16/561 (2.9%)
2	H	1.08	1/419 (0.2%)	2.00	16/561 (2.9%)
All	All	1.11	7/3208 (0.2%)	2.05	121/4300 (2.8%)

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	A	0	1
1	E	0	2
1	G	0	1
2	B	0	1
2	F	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	29	TYR	CA-CB	6.04	1.62	1.53
2	H	11	PHE	CA-CB	-5.85	1.44	1.53
1	A	13	VAL	CA-CB	5.76	1.61	1.54
1	G	4	ILE	CA-CB	5.19	1.61	1.54
1	A	44	PRO	CA-CB	-5.09	1.49	1.54
1	C	31	ARG	CZ-NH1	5.08	1.39	1.32
2	B	41	CYS	C-N	-5.04	1.26	1.33

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	44	PRO	O-C-N	12.28	126.96	121.31
1	G	31	ARG	NE-CZ-NH2	12.05	130.04	119.20
1	A	5	LYS	CA-CB-CG	10.49	135.08	114.10
1	C	31	ARG	CB-CG-CD	-10.24	87.76	111.30
2	B	28	GLN	CA-CB-CG	9.89	133.88	114.10
2	B	42	MET	N-CA-CB	-9.84	94.38	110.41
1	C	31	ARG	NE-CZ-NH2	-9.64	110.52	119.20
2	F	49	ASN	CA-CB-CG	9.62	122.22	112.60
2	F	49	ASN	OD1-CG-ND2	-9.49	113.11	122.60
2	B	28	GLN	N-CA-CB	-8.89	96.09	110.14
2	D	14	ASN	OD1-CG-ND2	-8.87	113.73	122.60
2	F	18	PHE	CA-CB-CG	8.73	122.53	113.80
1	E	13	VAL	CB-CA-C	-8.72	100.41	110.96
1	C	39	ASN	OD1-CG-ND2	-8.64	113.96	122.60
2	H	42	MET	N-CA-CB	-8.56	96.43	110.81
1	G	4	ILE	N-CA-C	-8.29	96.02	109.12
1	A	44	PRO	O-C-N	8.19	125.00	121.15
2	H	21	ASP	CA-CB-CG	8.05	120.65	112.60
1	G	31	ARG	NE-CZ-NH1	-7.89	113.61	121.50
2	B	34	PHE	CA-CB-CG	7.58	121.38	113.80
2	H	41	CYS	N-CA-C	-7.40	97.76	109.23
2	B	49	ASN	CA-CB-CG	7.39	119.99	112.60
2	B	42	MET	CA-CB-CG	7.34	128.78	114.10
2	B	7	ASP	CA-CB-CG	7.25	119.84	112.60
2	B	43	LYS	CA-CB-CG	7.19	128.49	114.10
1	E	26	GLU	O-C-N	-7.15	115.27	123.42
1	G	43	PRO	CB-CA-C	6.87	119.30	110.92
1	C	5	LYS	CA-CB-CG	-6.84	100.42	114.10
1	E	31	ARG	CG-CD-NE	-6.74	97.18	112.00
1	E	31	ARG	CB-CG-CD	6.72	126.76	111.30
2	D	42	MET	N-CA-CB	-6.68	100.28	110.77
1	E	8	GLU	CA-CB-CG	-6.67	100.76	114.10
1	E	4	ILE	N-CA-C	-6.63	98.49	108.17
2	F	43	LYS	CA-CB-CG	6.57	127.24	114.10
2	F	12	THR	CA-CB-OG1	-6.47	99.89	109.60
1	G	3	GLU	N-CA-C	-6.38	105.40	113.43
2	D	47	TYR	N-CA-C	6.33	124.28	110.80
1	A	5	LYS	N-CA-C	-6.31	97.35	110.80
2	F	5	ILE	N-CA-CB	-6.29	104.73	111.46
2	F	23	GLU	CB-CG-CD	6.22	123.17	112.60
1	G	43	PRO	CA-C-N	6.16	124.15	119.66
1	G	43	PRO	C-N-CA	6.16	124.15	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	G	44	PRO	CA-C-O	-6.11	116.50	120.90
2	B	42	MET	CB-CA-C	6.08	119.90	109.51
2	B	22	GLU	CA-CB-CG	-6.05	102.00	114.10
2	B	25	LYS	CB-CG-CD	-6.05	97.39	111.30
1	A	43	PRO	N-CA-C	-6.05	103.32	110.70
1	G	39	ASN	OD1-CG-ND2	-6.05	116.55	122.60
2	H	28	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	A	43	PRO	CA-C-N	6.04	124.01	119.66
1	A	43	PRO	C-N-CA	6.04	124.01	119.66
2	H	42	MET	CA-CB-CG	6.04	126.18	114.10
1	G	10	GLN	CB-CG-CD	5.96	122.73	112.60
2	B	24	ASN	OD1-CG-ND2	-5.94	116.66	122.60
2	F	13	GLN	OE1-CD-NE2	-5.94	116.66	122.60
2	B	42	MET	O-C-N	-5.86	116.49	123.06
2	F	49	ASN	N-CA-C	-5.86	100.16	109.59
2	H	49	ASN	OD1-CG-ND2	-5.85	116.75	122.60
2	H	43	LYS	CA-CB-CG	5.83	125.76	114.10
2	B	26	ILE	CA-C-N	5.83	132.83	121.41
2	B	26	ILE	C-N-CA	5.83	132.83	121.41
1	E	29	LYS	N-CA-C	5.83	117.43	111.14
1	G	36	LEU	CA-C-O	-5.77	112.96	120.00
2	B	3	TRP	CD2-CE2-CZ2	-5.75	116.65	122.40
2	B	3	TRP	CE2-CD2-CE3	5.71	124.52	118.80
1	C	3	GLU	CA-C-N	5.68	132.20	121.97
1	C	3	GLU	C-N-CA	5.68	132.20	121.97
2	D	2	GLU	N-CA-C	-5.68	103.03	110.53
2	D	40	PRO	CA-C-N	-5.67	113.74	122.87
2	D	40	PRO	C-N-CA	-5.67	113.74	122.87
1	C	27	ASP	CA-CB-CG	-5.66	106.94	112.60
1	C	3	GLU	N-CA-C	5.65	118.88	110.52
2	F	50	GLU	CA-CB-CG	5.64	125.38	114.10
1	E	13	VAL	N-CA-CB	5.63	117.42	111.00
2	H	24	ASN	OD1-CG-ND2	-5.62	116.98	122.60
2	F	49	ASN	CB-CG-ND2	5.59	124.79	116.40
1	C	39	ASN	CB-CG-ND2	5.56	124.75	116.40
1	G	24	ILE	CA-CB-CG1	-5.53	100.99	110.40
2	D	2	GLU	CB-CG-CD	5.53	122.00	112.60
2	D	24	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	G	5	LYS	CB-CG-CD	5.52	123.99	111.30
2	F	23	GLU	N-CA-C	-5.51	105.35	111.36
2	B	27	GLY	N-CA-C	5.50	126.22	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	3	GLU	CA-CB-CG	5.49	125.09	114.10
2	D	42	MET	CA-CB-CG	5.42	124.93	114.10
2	H	48	GLU	CB-CG-CD	5.41	121.79	112.60
2	H	42	MET	CB-CA-C	5.40	119.10	109.65
2	D	43	LYS	CA-CB-CG	5.39	124.88	114.10
2	F	14	ASN	CB-CA-C	-5.37	101.54	110.68
1	E	5	LYS	CA-CB-CG	-5.37	103.37	114.10
1	E	31	ARG	NE-CZ-NH1	5.36	126.86	121.50
2	H	8	ILE	N-CA-C	5.36	120.49	109.34
2	H	28	GLN	CG-CD-NE2	5.36	124.44	116.40
1	G	30	THR	O-C-N	5.33	129.48	122.33
2	H	1	GLY	N-CA-C	-5.33	97.85	113.30
1	C	11	LEU	CA-CB-CG	5.32	134.93	116.30
1	E	11	LEU	CA-CB-CG	5.32	134.91	116.30
2	H	26	ILE	O-C-N	-5.31	116.23	122.07
1	A	38	PHE	CA-CB-CG	5.30	119.10	113.80
2	B	11	PHE	N-CA-C	-5.30	105.42	111.14
1	G	6	GLY	CA-C-O	-5.30	116.46	121.60
1	A	8	GLU	N-CA-C	-5.28	99.99	108.55
2	H	46	ILE	N-CA-CB	-5.26	104.80	111.64
1	C	2	ARG	N-CA-C	-5.18	96.49	111.00
1	E	38	PHE	N-CA-C	-5.18	98.85	107.80
1	E	3	GLU	N-CA-C	-5.17	101.77	109.11
2	B	31	ARG	CA-C-O	-5.16	115.21	120.99
2	F	17	LYS	CA-C-O	-5.14	115.40	120.90
2	F	24	ASN	OD1-CG-ND2	-5.14	117.46	122.60
2	H	9	GLY	O-C-N	-5.13	117.80	122.42
2	D	3	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	E	20	PHE	CA-CB-CG	-5.11	108.69	113.80
1	C	38	PHE	CA-C-O	5.11	125.25	120.09
1	G	11	LEU	CB-CA-C	-5.09	100.06	109.37
1	E	31	ARG	NE-CZ-NH2	-5.08	114.63	119.20
1	A	34	LYS	CA-CB-CG	-5.08	103.94	114.10
1	G	31	ARG	CA-CB-CG	-5.05	103.99	114.10
1	A	3	GLU	N-CA-C	-5.05	101.64	109.72
1	A	2	ARG	CA-CB-CG	5.04	124.17	114.10
2	F	21	ASP	CA-CB-CG	5.03	117.63	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	TYR	Sidechain
2	B	29	TYR	Sidechain
1	E	3	GLU	Mainchain
1	E	31	ARG	Sidechain
2	F	29	TYR	Sidechain
1	G	7	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	A	373	0	371	16	0
1	C	373	0	371	10	0
1	E	373	0	371	5	0
1	G	373	0	371	10	0
2	B	411	0	407	13	0
2	D	411	0	407	10	0
2	F	411	0	407	5	0
2	H	411	0	407	13	0
All	All	3136	0	3112	63	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 10.

All (63) 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:F:42:MET:HE1	2:H:42:MET:SD	2.08	0.92
1:C:26:GLU:HG3	1:C:33:ARG:HG2	1.68	0.74
2:B:5:ILE:HD11	2:D:42:MET:HE1	1.69	0.72
1:G:10:GLN:NE2	2:H:3:TRP:HH2	1.88	0.71
1:A:3:GLU:HG2	1:A:5:LYS:HD3	1.73	0.70
1:G:2:ARG:HG2	1:G:29:LYS:NZ	2.08	0.69
2:B:6:ILE:HD11	2:B:41:CYS:SG	2.36	0.66
1:A:2:ARG:HD3	1:A:3:GLU:HB2	1.82	0.60
1:A:10:GLN:HB3	1:A:21:ARG:HH12	1.66	0.60
1:G:2:ARG:HG2	1:G:29:LYS:HZ2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:SER:OG	1:C:34:LYS:HB3	2.04	0.58
1:C:19:LEU:HD21	2:D:38:ILE:HD11	1.87	0.57
2:F:42:MET:CE	2:H:42:MET:SD	2.88	0.57
1:G:2:ARG:O	2:H:48:GLU:HB2	2.06	0.55
2:D:6:ILE:HG13	2:D:41:CYS:HB3	1.86	0.55
1:A:4:ILE:O	1:A:5:LYS:HD2	2.05	0.55
1:A:24:ILE:HD11	2:B:19:ALA:HB2	1.87	0.55
1:G:10:GLN:HE22	2:H:3:TRP:HH2	1.54	0.54
1:E:8:GLU:O	2:F:43:LYS:HA	2.10	0.52
1:A:23:ASP:O	1:A:36:LEU:HB2	2.09	0.52
2:H:16:GLY:O	2:H:20:VAL:HG23	2.10	0.52
1:C:40:GLY:HA2	1:C:42:VAL:HG13	1.92	0.51
2:D:18:PHE:CE1	2:D:22:GLU:HG3	2.46	0.51
2:D:3:TRP:CE3	2:D:42:MET:HE2	2.46	0.50
1:A:3:GLU:CG	1:A:5:LYS:HD3	2.40	0.49
2:F:5:ILE:HD11	2:H:42:MET:HE1	1.93	0.49
1:G:24:ILE:HD11	2:H:19:ALA:HB2	1.95	0.48
1:A:31:ARG:HG3	1:A:31:ARG:NH1	2.28	0.48
2:B:12:THR:HG23	2:B:41:CYS:SG	2.53	0.48
1:E:11:LEU:HD13	1:E:24:ILE:HD12	1.96	0.48
2:H:47:TYR:CD1	2:H:47:TYR:N	2.81	0.48
1:A:20:PHE:HE1	2:B:29:TYR:CE1	2.32	0.47
1:A:25:SER:HB3	1:A:36:LEU:HD11	1.97	0.47
1:C:23:ASP:O	1:C:36:LEU:HB2	2.14	0.47
2:B:16:GLY:HA3	2:B:34:PHE:HE2	1.78	0.46
2:H:3:TRP:CZ2	2:H:44:LYS:HD2	2.51	0.46
2:B:11:PHE:CE2	2:B:15:LEU:HD11	2.51	0.46
1:C:19:LEU:HD21	2:D:38:ILE:CD1	2.46	0.46
1:A:4:ILE:C	1:A:5:LYS:HD2	2.42	0.45
1:C:19:LEU:HD12	1:C:42:VAL:CG2	2.47	0.45
1:A:31:ARG:HG3	1:A:31:ARG:HH11	1.83	0.44
1:C:14:TYR:CZ	1:C:19:LEU:HD23	2.52	0.44
2:B:38:ILE:HD13	2:B:38:ILE:HG21	1.84	0.43
2:D:46:ILE:C	2:D:47:TYR:HD1	2.26	0.43
1:G:36:LEU:HA	1:G:36:LEU:HD23	1.81	0.43
2:H:26:ILE:O	2:H:28:GLN:N	2.52	0.43
1:E:34:LYS:HE2	1:E:36:LEU:HD23	2.01	0.43
1:C:31:ARG:HE	1:E:18:LYS:HE2	1.83	0.43
1:A:21:ARG:HA	1:A:21:ARG:HD2	1.85	0.43
1:A:10:GLN:HG2	1:A:21:ARG:HH22	1.84	0.42
1:G:3:GLU:HA	2:H:48:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HD12	2:B:49:ASN:N	2.33	0.42
2:D:45:THR:HG22	2:D:47:TYR:HE1	1.85	0.42
2:B:12:THR:HG22	2:B:37:VAL:HG11	2.02	0.41
2:B:3:TRP:HZ3	2:B:42:MET:HG3	1.85	0.41
2:D:23:GLU:O	2:D:26:ILE:N	2.53	0.41
1:E:10:GLN:NE2	2:F:3:TRP:HH2	2.18	0.41
1:C:9:TYR:HB3	1:C:11:LEU:CD1	2.49	0.41
1:G:14:TYR:CE2	2:H:38:ILE:HD13	2.55	0.41
1:A:3:GLU:CD	1:A:5:LYS:HD3	2.46	0.41
2:B:5:ILE:CD1	2:D:42:MET:HE1	2.47	0.40
2:B:3:TRP:CZ3	2:B:42:MET:HG3	2.57	0.40
1:G:36:LEU:O	1:G:37:ARG:HG3	2.21	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	42/44 (96%)	37 (88%)	4 (10%)	1 (2%)	4	17
1	C	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
1	E	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
1	G	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
2	B	48/50 (96%)	44 (92%)	1 (2%)	3 (6%)	1	3
2	D	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
2	F	48/50 (96%)	43 (90%)	5 (10%)	0	100	100
2	H	48/50 (96%)	44 (92%)	1 (2%)	3 (6%)	1	3
All	All	360/376 (96%)	329 (91%)	24 (7%)	7 (2%)	6	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	27	GLY
2	H	8	ILE
1	A	5	LYS
2	B	48	GLU
2	H	27	GLY
2	H	48	GLU
2	B	8	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	39/39 (100%)	35 (90%)	4 (10%)	7	23
1	C	39/39 (100%)	37 (95%)	2 (5%)	21	54
1	E	39/39 (100%)	34 (87%)	5 (13%)	4	15
1	G	39/39 (100%)	36 (92%)	3 (8%)	12	36
2	B	44/44 (100%)	37 (84%)	7 (16%)	2	9
2	D	44/44 (100%)	35 (80%)	9 (20%)	1	4
2	F	44/44 (100%)	36 (82%)	8 (18%)	2	6
2	H	44/44 (100%)	41 (93%)	3 (7%)	14	42
All	All	332/332 (100%)	291 (88%)	41 (12%)	4	16

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	5	LYS
1	A	19	LEU
1	A	26	GLU
2	B	2	GLU
2	B	5	ILE
2	B	22	GLU
2	B	26	ILE
2	B	28	GLN

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Mol	Chain	Res	Type
2	B	40	PRO
2	B	43	LYS
1	C	11	LEU
1	C	19	LEU
2	D	2	GLU
2	D	10	PRO
2	D	22	GLU
2	D	28	GLN
2	D	36	LYS
2	D	38	ILE
2	D	43	LYS
2	D	46	ILE
2	D	48	GLU
1	E	2	ARG
1	E	11	LEU
1	E	19	LEU
1	E	33	ARG
1	E	45	PRO
2	F	2	GLU
2	F	22	GLU
2	F	28	GLN
2	F	42	MET
2	F	43	LYS
2	F	44	LYS
2	F	48	GLU
2	F	49	ASN
1	G	3	GLU
1	G	19	LEU
1	G	30	THR
2	H	26	ILE
2	H	43	LYS
2	H	47	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	C	10	GLN
1	E	10	GLN
1	E	39	ASN
2	F	35	ASN
1	G	10	GLN

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Mol	Chain	Res	Type
2	H	35	ASN
2	H	49	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](#)

There are no ligands in this entry.

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.