



Full wwPDB NMR Structure Validation Report ⓘ

Mar 28, 2026 – 12:40 PM UTC

PDB ID : 1VRC / pdb_00001vrc
Title : Complex of enzyme IIamannose and the histidine-containing phosphocarrier protein HPr from escherichia coli nmr, restrained regularized mean structure
Authors : Clore, G.M.; Williams, D.C.
Deposited on : 2005-02-21

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

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)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

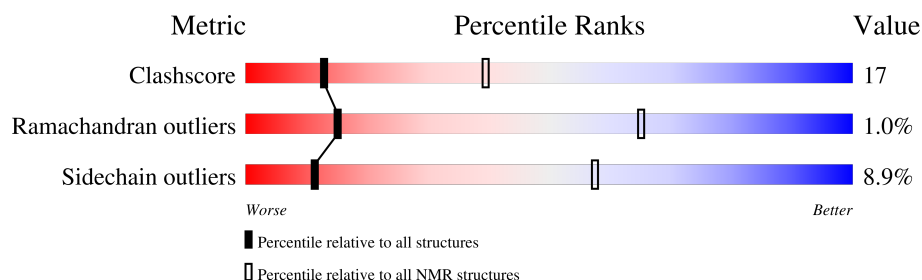
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	136	74% 17% . . 5%
1	B	136	74% 16% . . 5%
2	C	85	52% 34% 12% .
2	D	85	51% 34% 13% .

2 Ensemble composition and analysis ⓘ

This entry contains 2 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6542 atoms, of which 3284 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PTS system, mannose-specific IIAB component.

Mol	Chain	Residues	Atoms						Trace
1	A	129	Total	C	H	N	O	S	0
			1975	632	988	160	192	3	
1	B	129	Total	C	H	N	O	S	0
			1975	632	988	160	192	3	

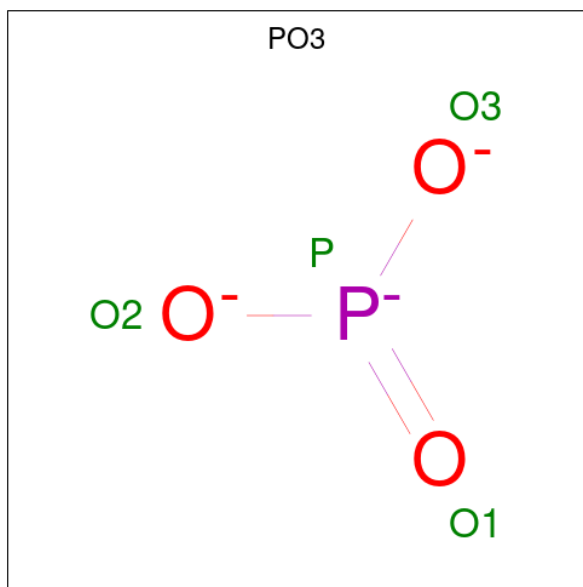
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P69797
A	134	PHE	-	cloning artifact	UNP P69797
A	135	ALA	-	cloning artifact	UNP P69797
A	136	GLY	-	cloning artifact	UNP P69797
B	1	MET	-	initiating methionine	UNP P69797
B	134	PHE	-	cloning artifact	UNP P69797
B	135	ALA	-	cloning artifact	UNP P69797
B	136	GLY	-	cloning artifact	UNP P69797

- Molecule 2 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						Trace
2	C	85	Total	C	H	N	O	S	0
			1292	401	654	107	128	2	
2	D	85	Total	C	H	N	O	S	0
			1292	401	654	107	128	2	

- Molecule 3 is PHOSPHITE ION (CCD ID: PO3) (formula: O₃P).



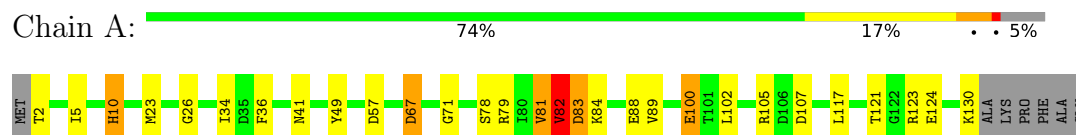
Mol	Chain	Residues	Atoms		
3	C	1	Total	O	P
			4	3	1
3	D	1	Total	O	P
			4	3	1

4 Residue-property plots

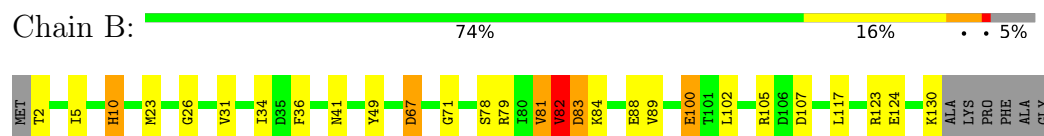
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

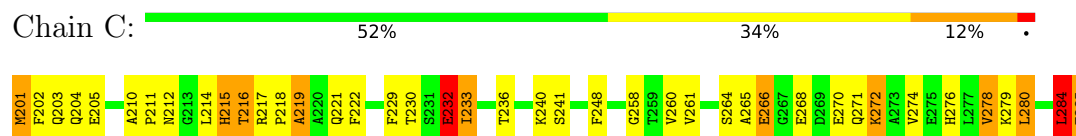
- Molecule 1: PTS system, mannose-specific IIAB component



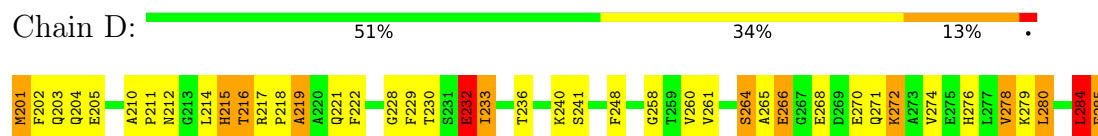
- Molecule 1: PTS system, mannose-specific IIAB component



- Molecule 2: Phosphocarrier protein HPr



- Molecule 2: Phosphocarrier protein HPr

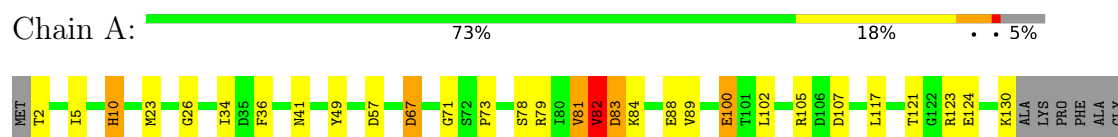


4.2 Scores per residue for each member of the ensemble

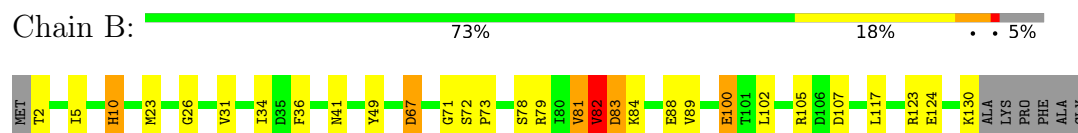
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

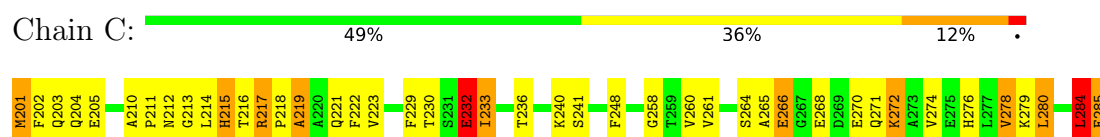
- Molecule 1: PTS system, mannose-specific IIAB component



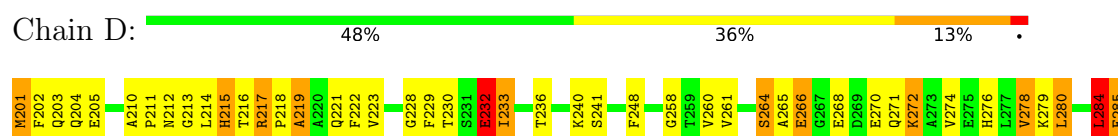
- Molecule 1: PTS system, mannose-specific IIAB component



- Molecule 2: Phosphocarrier protein HPr

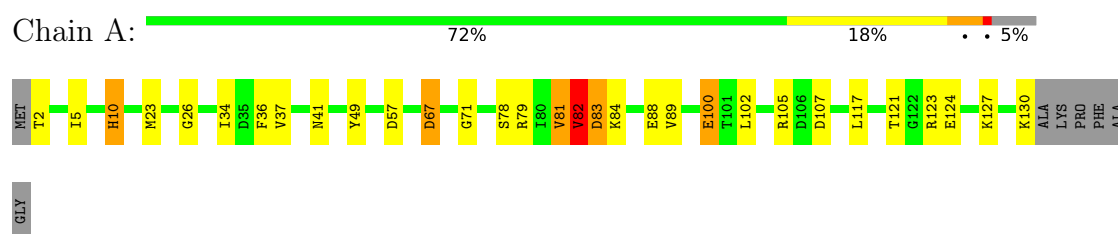


- Molecule 2: Phosphocarrier protein HPr

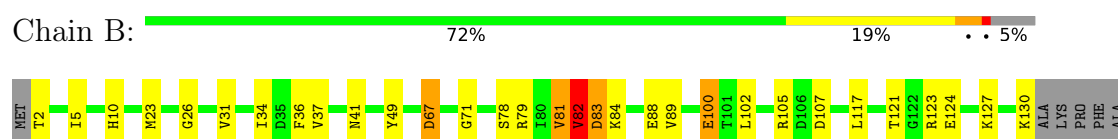


4.2.2 Score per residue for model 2

- Molecule 1: PTS system, mannose-specific IIAB component



- Molecule 1: PTS system, mannose-specific IIAB component



GLY

● Molecule 2: Phosphocarrier protein HPr



E285

● Molecule 2: Phosphocarrier protein HPr



L284
E285

5 Refinement protocol and experimental data overview

The models were refined using the following method: *CONJOINED RIGID BODY/TORSION ANGLE DYNAMICS*.

Of the 100 calculated structures, 2 were deposited, based on the following criterion: *REGULARIZED MEAN STRUCTURES*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	refinement	(HTTP://NMR.CIT.NIH.GOV/XPLOR_NIH)
X-PLOR NIH	structure solution	

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO3

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.86±0.03	0±0/1004 (0.0± 0.0%)	1.19±0.01	4±0/1366 (0.3± 0.0%)
1	B	0.86±0.03	0±0/1004 (0.0± 0.0%)	1.19±0.01	4±0/1366 (0.3± 0.0%)
2	C	1.58±0.01	3±0/645 (0.5± 0.0%)	2.14±0.00	33±0/870 (3.8± 0.0%)
2	D	1.58±0.01	4±0/645 (0.6± 0.0%)	2.14±0.00	35±0/870 (4.0± 0.0%)
All	All	1.19	14/6596 (0.2%)	1.63	153/8944 (1.7%)

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	C	260	VAL	C-O	8.36	1.33	1.24	1	2
2	D	260	VAL	C-O	8.25	1.33	1.24	1	2
2	D	212	ASN	N-CA	7.36	1.54	1.46	1	2
2	C	212	ASN	N-CA	7.27	1.54	1.46	1	2
2	D	221	GLN	CA-C	5.11	1.59	1.52	1	2
2	D	228	GLY	C-N	5.08	1.40	1.33	1	2
2	C	221	GLN	CA-C	5.04	1.59	1.52	1	2

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	270	GLU	N-CA-C	9.34	122.45	111.71	1	2
2	D	284	LEU	CA-C-O	8.57	130.30	120.96	1	2
2	D	270	GLU	N-CA-C	8.41	122.52	111.75	1	2
2	C	284	LEU	CA-C-O	8.33	130.42	120.92	1	2
2	D	284	LEU	CA-C-N	8.21	136.47	121.70	1	2
2	D	284	LEU	C-N-CA	8.21	136.47	121.70	1	2
2	C	284	LEU	CA-C-N	8.16	136.39	121.70	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	284	LEU	C-N-CA	8.16	136.39	121.70	1	2
2	D	268	GLU	CA-C-O	-7.96	112.12	120.55	1	2
2	C	268	GLU	CA-C-O	-7.90	112.18	120.55	1	2
2	D	214	LEU	CA-C-O	-7.78	112.92	122.64	2	1
2	C	214	LEU	CA-C-O	-7.74	112.97	122.64	2	1
2	C	222	PHE	CA-C-O	7.15	128.33	120.82	1	2
2	D	222	PHE	CA-C-O	7.11	128.28	120.82	1	2
2	C	280	LEU	CA-C-O	7.09	128.49	120.90	1	2
2	D	280	LEU	CA-C-O	7.03	128.42	120.90	1	2
2	C	265	ALA	O-C-N	6.96	131.59	123.17	1	2
2	D	265	ALA	O-C-N	6.96	131.59	123.17	1	2
2	D	261	VAL	O-C-N	6.88	129.92	122.76	1	2
2	C	261	VAL	O-C-N	6.82	129.85	122.76	1	2
2	D	210	ALA	CA-C-N	6.63	126.13	119.24	1	2
2	D	210	ALA	C-N-CA	6.63	126.13	119.24	1	2
2	C	210	ALA	CA-C-N	6.62	126.12	119.24	1	2
2	C	210	ALA	C-N-CA	6.62	126.12	119.24	1	2
1	B	67	ASP	N-CA-C	6.61	118.14	111.07	1	2
1	A	67	ASP	N-CA-C	6.55	118.07	111.07	1	2
2	D	241	SER	CA-C-O	6.52	129.08	121.46	1	2
2	C	241	SER	CA-C-O	6.46	129.02	121.46	1	2
2	C	274	VAL	O-C-N	6.39	128.07	121.87	1	2
2	D	274	VAL	O-C-N	6.37	128.04	121.87	1	2
2	C	278	VAL	O-C-N	6.34	128.36	121.83	1	2
2	D	278	VAL	O-C-N	6.32	128.34	121.83	1	2
2	C	280	LEU	O-C-N	-6.22	115.63	122.09	1	2
1	B	82	VAL	N-CA-C	6.16	122.16	109.34	1	2
2	D	280	LEU	O-C-N	-6.16	115.68	122.09	1	2
2	D	232	GLU	N-CA-C	-6.14	99.99	109.76	1	2
2	C	232	GLU	N-CA-C	-6.14	100.00	109.76	1	2
1	A	82	VAL	N-CA-C	6.13	122.09	109.34	1	2
2	C	213	GLY	O-C-N	-6.08	115.74	122.61	1	1
2	D	213	GLY	O-C-N	-6.07	115.75	122.61	1	1
2	D	261	VAL	CA-C-N	-6.05	114.65	123.00	1	2
2	D	261	VAL	C-N-CA	-6.05	114.65	123.00	1	2
2	C	261	VAL	CA-C-N	-6.01	114.70	123.00	1	2
2	C	261	VAL	C-N-CA	-6.01	114.70	123.00	1	2
2	C	211	PRO	CA-C-N	-5.99	113.61	122.83	1	2
2	C	211	PRO	C-N-CA	-5.99	113.61	122.83	1	2
2	D	211	PRO	CA-C-N	-5.93	113.70	122.83	1	2
2	D	211	PRO	C-N-CA	-5.93	113.70	122.83	1	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	C	216	THR	N-CA-C	5.78	120.85	111.37	2	1
2	D	236	THR	CA-C-N	-5.78	114.63	122.77	1	2
2	D	236	THR	C-N-CA	-5.78	114.63	122.77	1	2
2	C	240	LYS	N-CA-C	-5.75	100.03	109.40	1	2
2	C	219	ALA	O-C-N	-5.74	115.60	122.15	1	2
2	C	236	THR	CA-C-N	-5.74	114.68	122.77	1	2
2	C	236	THR	C-N-CA	-5.74	114.68	122.77	1	2
2	D	212	ASN	N-CA-C	-5.74	106.08	112.57	1	2
2	D	240	LYS	N-CA-C	-5.71	100.09	109.40	1	2
1	B	26	GLY	N-CA-C	-5.71	105.42	112.33	1	2
2	D	216	THR	N-CA-C	5.71	120.73	111.37	2	1
2	C	230	THR	CA-C-O	-5.70	113.07	119.79	1	2
1	A	26	GLY	N-CA-C	-5.69	105.44	112.33	1	2
2	D	219	ALA	O-C-N	-5.67	115.69	122.15	1	2
2	D	230	THR	CA-C-O	-5.66	113.11	119.79	1	2
2	C	212	ASN	N-CA-C	-5.65	106.19	112.57	1	2
2	D	217	ARG	O-C-N	-5.40	116.12	120.38	1	1
2	C	265	ALA	CA-C-N	-5.36	114.67	122.44	1	2
2	C	265	ALA	C-N-CA	-5.36	114.67	122.44	1	2
2	C	217	ARG	O-C-N	-5.35	116.15	120.38	1	1
2	D	265	ALA	CA-C-N	-5.33	114.71	122.44	1	2
2	D	265	ALA	C-N-CA	-5.33	114.71	122.44	1	2
1	B	23	MET	N-CA-C	-5.32	105.65	111.82	1	2
2	C	258	GLY	CA-C-O	5.29	124.98	119.06	1	2
1	A	23	MET	N-CA-C	-5.29	105.69	111.82	1	2
2	D	258	GLY	CA-C-O	5.28	124.97	119.06	1	2
2	C	233	ILE	O-C-N	5.23	128.69	123.10	1	2
2	D	272	LYS	N-CA-C	-5.20	105.61	111.28	1	2
2	C	272	LYS	N-CA-C	-5.19	105.62	111.28	1	2
2	D	233	ILE	O-C-N	5.18	128.64	123.10	1	2
2	D	264	SER	CA-C-N	-5.04	114.04	122.21	1	2
2	D	264	SER	C-N-CA	-5.04	114.04	122.21	1	2
1	A	10	HIS	N-CA-C	-5.02	103.43	110.50	2	1

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	987	988	986	32±0
1	B	987	988	986	32±0
2	C	638	654	650	28±2
2	D	638	654	650	30±2
3	C	0	0	0	4±4
3	D	0	0	0	3±3
All	All	6508	6568	6544	216

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 17.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:215:HIS:ND1	3:C:401:PO3:P	1.34	2.01	1	1
2:D:215:HIS:ND1	3:D:400:PO3:P	1.34	2.00	1	1
2:C:232:GLU:CD	2:C:232:GLU:C	1.13	2.16	1	2
2:D:232:GLU:CD	2:D:232:GLU:C	1.11	2.16	1	2
1:A:123:ARG:HH21	1:B:123:ARG:NH2	1.01	1.53	1	2
1:A:123:ARG:NH2	1:B:123:ARG:HH21	1.00	1.52	1	2
2:C:232:GLU:O	2:C:232:GLU:OE2	0.90	1.88	1	2
2:D:232:GLU:O	2:D:232:GLU:OE2	0.90	1.89	1	2
1:A:123:ARG:HH21	1:B:123:ARG:HH21	0.87	0.90	1	2
1:B:100:GLU:OE1	1:B:117:LEU:HD21	0.84	1.73	2	2
2:D:232:GLU:C	2:D:232:GLU:OE2	0.83	2.22	1	2
2:C:232:GLU:C	2:C:232:GLU:OE2	0.82	2.22	1	2
1:B:10:HIS:ND1	1:B:67:ASP:OD2	0.80	2.14	2	1
1:A:10:HIS:ND1	1:A:67:ASP:OD2	0.80	2.13	2	1
2:C:272:LYS:NZ	2:C:276:HIS:CE1	0.74	2.55	1	2
2:D:272:LYS:NZ	2:D:276:HIS:CE1	0.74	2.56	1	2
2:D:215:HIS:CE1	3:D:400:PO3:P	0.73	2.81	1	1
2:C:215:HIS:CE1	3:C:401:PO3:P	0.73	2.82	1	1
1:A:100:GLU:OE1	1:A:117:LEU:HD21	0.72	1.84	2	2
1:A:78:SER:O	1:A:82:VAL:HG13	0.71	1.86	1	2
1:B:78:SER:O	1:B:82:VAL:HG13	0.70	1.86	1	2
1:B:100:GLU:OE1	1:B:117:LEU:CD2	0.69	2.41	2	2
1:A:102:LEU:CD2	1:A:105:ARG:NH2	0.67	2.58	1	2
1:A:124:GLU:OE1	2:C:248:PHE:CE2	0.66	2.49	2	2
1:B:124:GLU:OE1	2:D:248:PHE:CE2	0.66	2.48	2	2
2:C:232:GLU:CD	2:C:233:ILE:N	0.66	2.54	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:232:GLU:CD	2:D:233:ILE:N	0.65	2.54	1	2
1:A:123:ARG:NH2	1:B:123:ARG:NH2	0.65	2.27	1	2
1:B:102:LEU:CD2	1:B:105:ARG:NH2	0.65	2.60	1	2
1:A:100:GLU:CD	1:A:121:THR:HG21	0.63	2.18	2	1
1:A:100:GLU:OE1	1:A:117:LEU:CD2	0.60	2.49	2	1
2:C:232:GLU:CD	2:C:232:GLU:O	0.59	2.38	1	2
2:C:280:LEU:HG	2:C:284:LEU:CD2	0.58	2.28	1	2
1:B:2:THR:HB	1:B:105:ARG:CD	0.58	2.27	1	2
2:D:280:LEU:HG	2:D:284:LEU:CD2	0.58	2.28	1	2
1:A:100:GLU:OE1	1:A:121:THR:HG21	0.58	1.99	2	2
2:D:280:LEU:O	2:D:284:LEU:HD22	0.57	1.99	1	2
1:A:2:THR:HB	1:A:105:ARG:CD	0.57	2.28	1	2
1:A:102:LEU:CD2	1:A:105:ARG:HH21	0.57	2.11	1	2
1:B:5:ILE:HD12	1:B:105:ARG:HH21	0.57	1.59	1	2
2:C:280:LEU:O	2:C:284:LEU:HD22	0.57	1.99	1	2
2:D:285:GLU:H	2:D:285:GLU:CD	0.56	2.08	1	2
1:A:130:LYS:HE3	1:B:81:VAL:HG23	0.56	1.78	1	2
1:A:107:ASP:OD1	1:A:107:ASP:C	0.55	2.49	2	2
1:B:36:PHE:C	1:B:36:PHE:CD1	0.55	2.84	2	2
1:A:36:PHE:C	1:A:36:PHE:CD1	0.55	2.84	2	2
2:C:272:LYS:HZ2	2:C:276:HIS:CE1	0.55	2.18	1	2
1:B:10:HIS:CE1	1:B:73:PRO:HD2	0.55	2.37	1	1
1:A:10:HIS:CE1	1:A:73:PRO:HD2	0.54	2.37	1	1
1:B:107:ASP:OD1	1:B:107:ASP:C	0.54	2.49	2	2
2:D:272:LYS:HZ2	2:D:276:HIS:CE1	0.54	2.19	1	2
1:A:81:VAL:HG23	1:B:130:LYS:HE3	0.54	1.79	1	2
1:A:71:GLY:CA	2:D:216:THR:OG1	0.54	2.56	1	2
1:B:71:GLY:CA	2:C:216:THR:OG1	0.53	2.56	1	2
1:B:100:GLU:CD	1:B:121:THR:HG21	0.53	2.28	2	1
2:D:247:LEU:O	2:D:251:GLN:HG3	0.53	2.03	2	1
1:B:100:GLU:OE1	1:B:117:LEU:CG	0.53	2.57	2	1
1:B:102:LEU:CD2	1:B:105:ARG:HH21	0.53	2.17	1	2
2:C:247:LEU:O	2:C:251:GLN:HG3	0.53	2.03	2	1
1:A:5:ILE:HD12	1:A:105:ARG:HH21	0.52	1.64	1	2
1:A:100:GLU:OE1	1:A:117:LEU:CG	0.52	2.57	2	1
1:A:83:ASP:N	1:A:83:ASP:OD1	0.51	2.43	1	2
2:C:272:LYS:HZ1	2:C:276:HIS:CE1	0.51	2.23	1	2
2:C:280:LEU:HG	2:C:284:LEU:HD21	0.51	1.83	1	2
2:D:280:LEU:HG	2:D:284:LEU:HD21	0.51	1.83	1	2
2:D:219:ALA:O	2:D:223:VAL:HG23	0.50	2.07	1	1
2:C:203:GLN:O	2:C:204:GLN:HG2	0.50	2.07	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:D:272:LYS:HZ1	2:D:276:HIS:CE1	0.50	2.22	1	2
1:B:124:GLU:OE1	2:D:248:PHE:CZ	0.50	2.64	2	1
2:D:203:GLN:O	2:D:204:GLN:HG2	0.50	2.07	1	2
1:A:124:GLU:OE1	2:C:248:PHE:CZ	0.50	2.63	2	1
2:C:285:GLU:H	2:C:285:GLU:CD	0.50	2.08	1	2
2:C:219:ALA:O	2:C:223:VAL:HG23	0.49	2.06	1	1
2:D:232:GLU:CD	2:D:232:GLU:O	0.49	2.38	1	2
2:C:203:GLN:C	2:C:204:GLN:HG2	0.49	2.32	1	2
2:D:215:HIS:CE1	2:D:218:PRO:HD3	0.48	2.43	2	2
2:C:215:HIS:CE1	2:C:218:PRO:HD3	0.48	2.43	2	2
1:B:10:HIS:CE1	1:B:73:PRO:CD	0.48	2.96	1	1
1:B:83:ASP:N	1:B:83:ASP:OD1	0.48	2.44	1	2
1:A:10:HIS:CE1	1:A:73:PRO:CD	0.48	2.96	1	1
1:B:2:THR:HB	1:B:105:ARG:HD3	0.48	1.84	1	2
2:D:203:GLN:C	2:D:204:GLN:HG2	0.48	2.32	1	2
2:C:272:LYS:O	2:C:276:HIS:CD2	0.48	2.67	1	2
1:A:82:VAL:HG23	1:A:83:ASP:OD1	0.48	2.09	1	2
2:D:272:LYS:O	2:D:276:HIS:CD2	0.48	2.67	1	2
1:B:82:VAL:HG23	1:B:83:ASP:OD1	0.47	2.10	1	2
2:C:201:MET:CG	2:C:202:PHE:N	0.46	2.78	1	2
1:B:124:GLU:OE1	2:D:248:PHE:CD2	0.46	2.68	2	2
2:D:215:HIS:ND1	3:D:400:PO3:O1	0.46	2.47	1	1
1:A:2:THR:HB	1:A:105:ARG:HD3	0.45	1.88	1	2
1:A:124:GLU:OE1	2:C:248:PHE:CD2	0.45	2.68	2	2
1:B:88:GLU:HG3	1:B:89:VAL:N	0.45	2.26	1	2
2:D:201:MET:CG	2:D:202:PHE:N	0.45	2.79	1	2
2:D:229:PHE:HE1	2:D:272:LYS:HE3	0.45	1.71	1	2
1:A:34:ILE:HG12	1:A:49:TYR:CE1	0.45	2.47	1	2
2:C:229:PHE:HE1	2:C:272:LYS:HE3	0.45	1.71	1	2
1:A:88:GLU:HG3	1:A:89:VAL:N	0.45	2.26	1	2
2:C:215:HIS:ND1	3:C:401:PO3:O3	0.44	2.47	1	1
2:C:215:HIS:ND1	3:C:401:PO3:O1	0.44	2.47	1	1
1:B:100:GLU:OE1	1:B:121:THR:HG21	0.44	2.13	2	1
2:D:214:LEU:O	2:D:215:HIS:O	0.44	2.36	1	1
1:A:71:GLY:HA2	3:D:400:PO3:O1	0.43	2.13	1	1
2:C:214:LEU:O	2:C:215:HIS:O	0.43	2.36	1	1
1:B:36:PHE:CD1	1:B:37:VAL:N	0.43	2.87	2	1
1:B:34:ILE:HG12	1:B:49:TYR:CE1	0.43	2.49	1	2
2:D:215:HIS:ND1	3:D:400:PO3:O3	0.43	2.47	1	1
2:D:201:MET:HG3	2:D:202:PHE:N	0.42	2.29	1	2
1:B:71:GLY:HA2	3:C:401:PO3:O1	0.42	2.13	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:201:MET:HG3	2:C:202:PHE:N	0.42	2.29	1	2
1:A:36:PHE:CD1	1:A:37:VAL:N	0.42	2.87	2	1
1:A:67:ASP:N	1:A:67:ASP:OD1	0.42	2.52	1	2
1:B:67:ASP:N	1:B:67:ASP:OD1	0.42	2.53	1	2
1:A:102:LEU:HD23	1:A:105:ARG:HH21	0.42	1.72	1	2
2:C:215:HIS:CE1	2:C:218:PRO:CD	0.42	3.03	2	1
2:D:215:HIS:CE1	2:D:218:PRO:CD	0.42	3.03	2	1
1:A:79:ARG:O	1:A:82:VAL:HG22	0.42	2.14	1	2
1:B:31:VAL:CG2	1:B:105:ARG:HH22	0.41	2.28	1	2
2:D:217:ARG:N	3:D:400:PO3:O3	0.41	2.50	1	1
1:A:100:GLU:OE1	1:A:117:LEU:HD11	0.41	2.15	1	1
2:C:217:ARG:N	3:C:401:PO3:O3	0.41	2.51	1	1
1:B:72:SER:N	3:C:401:PO3:O1	0.41	2.53	1	1
2:D:201:MET:HB2	2:D:266:GLU:HG2	0.41	1.92	1	2
1:A:124:GLU:CD	2:C:248:PHE:CZ	0.41	2.98	1	1
2:D:284:LEU:HD12	2:D:284:LEU:HA	0.41	1.57	1	2
1:B:79:ARG:O	1:B:82:VAL:HG22	0.41	2.14	1	2
1:A:57:ASP:OD1	1:A:57:ASP:C	0.41	2.64	1	2
1:B:124:GLU:CD	2:D:248:PHE:CZ	0.40	2.98	1	1
2:C:201:MET:HB2	2:C:266:GLU:HG2	0.40	1.92	1	2

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	127/136 (93%)	126±0 (99±0%)	0±0 (0±0%)	2±0 (1±0%)	13	61
1	B	127/136 (93%)	126±0 (99±0%)	0±0 (0±0%)	2±0 (1±0%)	13	61
2	C	83/85 (98%)	80±0 (97±1%)	2±1 (2±1%)	0±0 (1±1%)	23	72
2	D	83/85 (98%)	80±0 (97±1%)	2±1 (2±1%)	0±0 (1±1%)	23	72
All	All	840/884 (95%)	824 (98%)	8 (1%)	8 (1%)	15	65

All 6 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	82	VAL	2
1	B	82	VAL	2
1	A	10	HIS	1
1	B	10	HIS	1
2	C	215	HIS	1
2	D	215	HIS	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. 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	104/108 (96%)	98±0 (95±0%)	6±0 (5±0%)	22 72
1	B	104/108 (96%)	98±0 (95±0%)	6±0 (5±0%)	22 72
2	C	70/70 (100%)	60±0 (86±0%)	10±0 (14±0%)	5 44
2	D	70/70 (100%)	60±0 (86±0%)	10±0 (14±0%)	5 44
All	All	696/712 (98%)	634 (91%)	62 (9%)	11 57

All 32 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	41	ASN	2
1	A	81	VAL	2
1	A	83	ASP	2
1	A	84	LYS	2
1	A	100	GLU	2
1	B	41	ASN	2
1	B	81	VAL	2
1	B	83	ASP	2
1	B	84	LYS	2
1	B	100	GLU	2
2	C	201	MET	2
2	C	205	GLU	2
2	C	232	GLU	2
2	C	264	SER	2
2	C	266	GLU	2
2	C	271	GLN	2

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Mol	Chain	Res	Type	Models (Total)
2	C	278	VAL	2
2	C	279	LYS	2
2	C	284	LEU	2
2	C	285	GLU	2
2	D	201	MET	2
2	D	205	GLU	2
2	D	232	GLU	2
2	D	264	SER	2
2	D	266	GLU	2
2	D	271	GLN	2
2	D	278	VAL	2
2	D	279	LYS	2
2	D	284	LEU	2
2	D	285	GLU	2
1	A	127	LYS	1
1	B	127	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
3	PO3	C	401	-	0,3,3	0.00±0.00	-
3	PO3	D	400	-	0,3,3	0.00±0.00	-

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
3	PO3	C	401	-	0,3,3	0.00±0.00	-
3	PO3	D	400	-	0,3,3	0.00±0.00	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided