



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:43 PM UTC

PDB ID : 1O9R / pdb_00001o9r
Title : The X-ray crystal structure of Agrobacterium tumefaciens Dps, a member of the family that protect DNA without binding
Authors : Ilari, A.; Ceci, P.; Chiancone, E.
Deposited on : 2002-12-18
Resolution : 1.45 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:

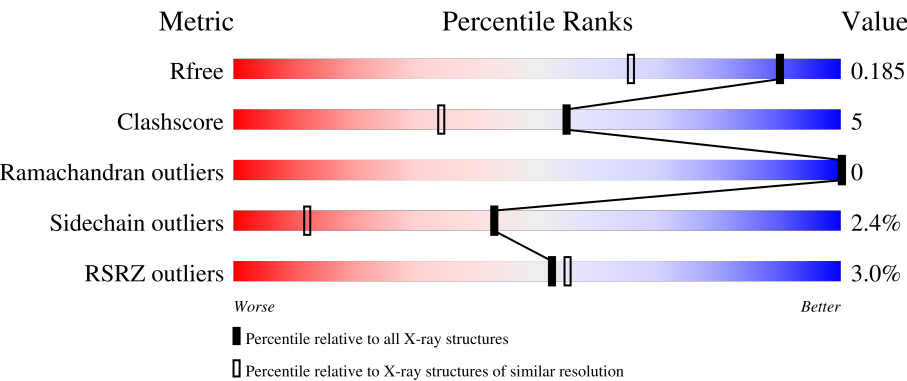
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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))
R _{free}	180053	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	162	2% 85% 13% ..
1	B	162	2% 80% 19% .
1	C	162	4% 83% 12% ..
1	D	162	3% 86% 7% 5% ..
1	E	162	4% 86% 12% .

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Mol	Chain	Length	Quality of chain
1	F	162	3% 85% 12% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8286 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 AGROBACTERIUM TUMEFACIENS DPS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	1	0
			1260	790	217	251	2			
1	B	162	Total	C	N	O	S	0	1	0
			1260	790	217	251	2			
1	C	159	Total	C	N	O	S	0	1	0
			1236	775	213	247	1			
1	D	160	Total	C	N	O	S	0	1	0
			1243	779	214	249	1			
1	E	162	Total	C	N	O	S	0	1	0
			1260	790	217	251	2			
1	F	162	Total	C	N	O	S	0	1	0
			1260	790	217	251	2			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			8	4	1	3		
3	E	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		

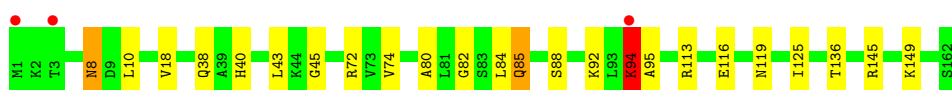
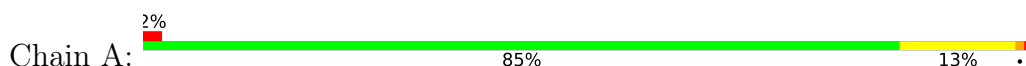
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	129	Total 129	O 129	0	0
5	B	134	Total 134	O 134	0	0
5	C	121	Total 121	O 121	0	0
5	D	115	Total 115	O 115	0	0
5	E	116	Total 116	O 116	0	0
5	F	126	Total 126	O 126	0	0

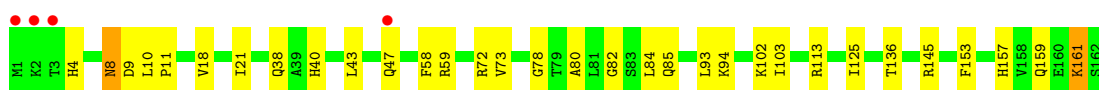
3 Residue-property plots [i](#)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

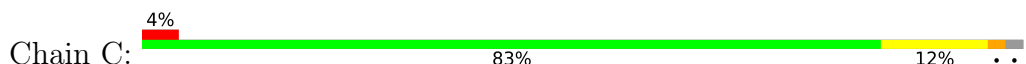
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS



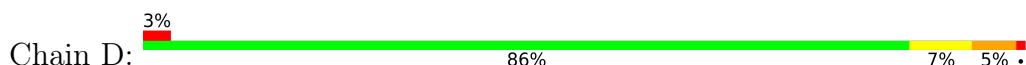
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS



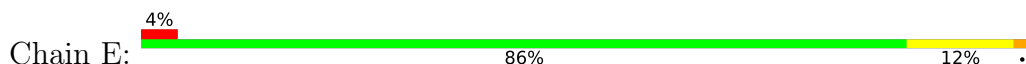
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS



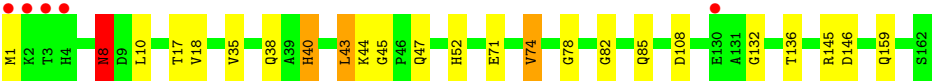
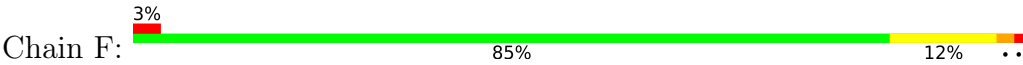
- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS



- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS



- Molecule 1: AGROBACTERIUM TUMEFACIENS DPS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.05Å 90.35Å 105.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.45 20.00 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-1.45) 96.3 (20.00-1.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.19 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.170 , 0.200 (Not available) , 0.185	Depositor DCC
R_{free} test set	8603 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8286	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5536e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.11	0/1285	1.71	17/1742 (1.0%)
1	B	1.13	0/1285	1.75	24/1742 (1.4%)
1	C	1.09	1/1261 (0.1%)	1.67	18/1711 (1.1%)
1	D	1.14	0/1268	1.78	17/1721 (1.0%)
1	E	1.13	0/1285	1.73	17/1742 (1.0%)
1	F	1.09	0/1285	1.67	15/1742 (0.9%)
All	All	1.12	1/7669 (0.0%)	1.72	108/10400 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	GLY	N-CA	5.65	1.50	1.44

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	13	ASN	OD1-CG-ND2	9.68	132.28	122.60
1	B	161	LYS	CD-CE-NZ	9.59	142.59	111.90
1	C	159	GLN	OE1-CD-NE2	-9.17	113.43	122.60
1	D	159	GLN	OE1-CD-NE2	-8.84	113.77	122.60
1	F	159	GLN	OE1-CD-NE2	-8.75	113.85	122.60
1	E	43	LEU	CA-CB-CG	8.33	145.44	116.30
1	A	125	ILE	O-C-N	8.10	129.85	121.91
1	D	161	LYS	CA-C-N	-7.79	107.67	121.70
1	D	161	LYS	C-N-CA	-7.79	107.67	121.70
1	D	86	ALA	CA-C-O	7.62	128.62	120.55
1	B	125	ILE	O-C-N	7.34	129.11	121.91
1	C	40	HIS	CA-CB-CG	7.28	121.08	113.80
1	F	132	GLY	CA-C-N	-7.22	114.28	123.16
1	F	132	GLY	C-N-CA	-7.22	114.28	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	ARG	NE-CZ-NH1	7.21	128.71	121.50
1	E	145	ARG	CD-NE-CZ	-7.07	114.51	124.40
1	B	159	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	D	38	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	E	43	LEU	CB-CA-C	-6.90	97.86	109.65
1	E	159	GLN	OE1-CD-NE2	-6.82	115.78	122.60
1	E	158	VAL	CA-C-O	-6.82	113.45	119.38
1	D	40	HIS	CA-CB-CG	6.82	120.62	113.80
1	F	40	HIS	CA-CB-CG	6.72	120.52	113.80
1	B	78	GLY	O-C-N	6.69	129.24	122.88
1	B	84	LEU	O-C-N	6.56	129.07	122.12
1	F	47	GLN	CG-CD-NE2	6.52	126.18	116.40
1	C	77	GLY	CA-C-N	-6.50	116.64	122.43
1	C	77	GLY	C-N-CA	-6.50	116.64	122.43
1	E	9	ASP	CA-CB-CG	6.39	118.99	112.60
1	B	59	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	A	94	LYS	CA-CB-CG	6.27	126.65	114.10
1	A	40	HIS	CA-CB-CG	6.19	119.99	113.80
1	F	47	GLN	OE1-CD-NE2	-6.15	116.45	122.60
1	A	74	VAL	CA-CB-CG2	6.13	120.81	110.40
1	A	45	GLY	CA-C-N	6.11	125.80	119.56
1	A	45	GLY	C-N-CA	6.11	125.80	119.56
1	C	75	GLN	CA-C-O	-6.08	113.23	120.10
1	E	75	GLN	CA-C-O	-6.05	113.26	120.10
1	B	43	LEU	CB-CA-C	-6.02	99.72	109.72
1	B	113	ARG	NE-CZ-NH2	-5.98	113.81	119.20
1	E	131	ALA	CA-C-N	5.95	129.71	121.26
1	E	131	ALA	C-N-CA	5.95	129.71	121.26
1	A	94	LYS	CB-CG-CD	5.95	124.97	111.30
1	C	145	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	F	78	GLY	O-C-N	5.87	128.45	122.88
1	D	129	ASP	CA-CB-CG	-5.85	106.75	112.60
1	B	93	LEU	O-C-N	5.82	129.91	123.16
1	A	72	ARG	CA-C-O	-5.78	114.30	120.42
1	B	80	ALA	CA-C-O	-5.75	114.72	121.16
1	E	19	ILE	O-C-N	-5.75	116.30	121.87
1	E	13	ASN	CB-CG-ND2	-5.70	107.85	116.40
1	B	145	ARG	CD-NE-CZ	-5.68	116.44	124.40
1	D	126	ASP	CA-C-O	-5.67	114.42	120.42
1	F	74	VAL	CA-CB-CG2	5.65	120.00	110.40
1	A	119	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	F	17	THR	O-C-N	5.61	127.85	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	LYS	CG-CD-CE	5.59	124.16	111.30
1	D	52	HIS	CB-CG-CD2	-5.59	123.93	131.20
1	C	11	PRO	CA-C-N	5.59	128.03	120.38
1	C	11	PRO	C-N-CA	5.59	128.03	120.38
1	C	75	GLN	O-C-N	5.59	128.76	122.22
1	B	40	HIS	CA-CB-CG	5.57	119.37	113.80
1	E	145	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	F	145	ARG	CD-NE-CZ	-5.55	116.62	124.40
1	A	88	SER	CA-C-O	-5.51	114.71	120.55
1	E	145	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	B	58	PHE	CA-CB-CG	5.50	119.30	113.80
1	D	40	HIS	CG-CD2-NE2	5.50	112.70	107.20
1	A	92	LYS	CG-CD-CE	5.50	123.95	111.30
1	E	17	THR	O-C-N	5.48	127.72	122.07
1	A	80	ALA	O-C-N	5.48	129.67	122.93
1	D	86	ALA	O-C-N	-5.47	116.32	122.12
1	B	59	ARG	NE-CZ-NH1	-5.46	116.03	121.50
1	C	86	ALA	CA-C-O	5.46	126.20	120.42
1	D	59	ARG	NE-CZ-NH2	5.45	124.10	119.20
1	F	45	GLY	CA-C-N	5.42	124.94	119.19
1	F	45	GLY	C-N-CA	5.42	124.94	119.19
1	E	64	ASN	CA-CB-CG	-5.42	107.18	112.60
1	B	84	LEU	CA-C-O	-5.40	114.79	120.63
1	A	149	LYS	CA-C-O	-5.39	114.70	120.42
1	F	108	ASP	CA-C-O	5.38	126.47	120.82
1	A	145	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	F	146	ASP	CA-CB-CG	-5.31	107.29	112.60
1	C	6	THR	N-CA-CB	5.30	120.61	111.13
1	E	52	HIS	CA-CB-CG	5.30	119.10	113.80
1	B	9	ASP	CA-C-O	-5.28	113.50	119.78
1	C	59	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	D	162	SER	CB-CA-C	5.26	120.10	110.10
1	B	72	ARG	CA-C-O	-5.25	114.86	120.42
1	D	145	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	D	126	ASP	O-C-N	5.24	128.12	122.15
1	D	153	PHE	CA-CB-CG	5.23	119.03	113.80
1	B	11	PRO	N-CA-CB	-5.22	98.93	103.32
1	C	17	THR	CA-CB-OG1	-5.22	101.77	109.60
1	A	95	ALA	CA-C-O	5.18	126.61	120.96
1	B	73	VAL	O-C-N	-5.15	116.79	121.94
1	B	4	HIS	CA-CB-CG	-5.14	108.66	113.80
1	B	21	ILE	O-C-N	5.13	126.94	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	137	ALA	CA-C-O	-5.13	114.31	120.10
1	C	132	GLY	CA-C-N	-5.09	116.90	123.16
1	C	132	GLY	C-N-CA	-5.09	116.90	123.16
1	A	84	LEU	O-C-N	5.08	127.51	122.12
1	C	99	ASP	CA-CB-CG	-5.08	107.52	112.60
1	F	8	ASN	CA-C-O	-5.04	115.36	120.80
1	B	103	ILE	CA-C-O	-5.04	115.71	120.95
1	C	6	THR	CA-CB-CG2	5.04	119.06	110.50
1	D	13	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	43	LEU	CB-CA-C	-5.01	101.08	109.65

There are no chirality outliers.

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	1260	0	1255	19	0
1	B	1260	0	1255	13	0
1	C	1236	0	1223	12	0
1	D	1243	0	1230	11	0
1	E	1260	0	1255	14	0
1	F	1260	0	1255	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	B	8	0	12	0	0
3	E	8	0	12	0	0
4	D	4	0	5	0	0
5	A	129	0	0	0	0
5	B	134	0	0	0	0
5	C	121	0	0	0	1
5	D	115	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	116	0	0	0	0
5	F	126	0	0	0	0
All	All	8286	0	7502	72	1

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 5.

All (72) 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:94:LYS:NZ	1:A:113:ARG:HG2	1.88	0.89
1:A:94:LYS:HE3	1:A:94:LYS:H	1.39	0.84
1:A:94:LYS:HZ3	1:A:113:ARG:HG2	1.44	0.82
1:A:38:GLN:HE22	1:B:82:GLY:H	1.31	0.78
1:E:82:GLY:H	1:F:38:GLN:HE22	1.34	0.76
1:A:94:LYS:H	1:A:94:LYS:CE	1.99	0.75
1:A:38:GLN:NE2	1:B:82:GLY:H	1.86	0.74
1:A:82:GLY:H	1:B:38:GLN:HE22	1.34	0.73
1:E:38:GLN:HE22	1:F:82:GLY:H	1.37	0.71
1:A:82:GLY:H	1:B:38:GLN:NE2	1.91	0.69
1:E:82:GLY:H	1:F:38:GLN:NE2	1.92	0.67
1:E:38:GLN:NE2	1:F:82:GLY:H	1.94	0.64
1:D:94:LYS:HE3	1:D:94:LYS:HA	1.80	0.63
1:A:94:LYS:NZ	1:A:116:GLU:OE2	2.32	0.63
1:D:43:LEU:HD12	1:D:43:LEU:H	1.67	0.59
1:A:94:LYS:HZ3	1:A:113:ARG:CG	2.16	0.58
1:A:94:LYS:HZ2	1:A:113:ARG:HG2	1.65	0.57
1:C:94:LYS:N	1:C:94:LYS:HD3	2.19	0.56
1:C:8:ASN:C	1:C:8:ASN:HD22	2.14	0.56
1:C:94:LYS:NZ	1:C:94:LYS:H	2.04	0.56
1:D:59:ARG:NH1	5:D:2039:HOH:O	2.39	0.54
1:B:18:VAL:CG1	1:B:136:THR:HG21	2.38	0.53
1:A:8:ASN:C	1:A:8:ASN:HD22	2.16	0.53
1:D:8:ASN:HD22	1:D:8:ASN:C	2.18	0.52
1:C:94:LYS:H	1:C:94:LYS:HZ2	1.58	0.52
1:F:8:ASN:HD22	1:F:10:LEU:H	1.58	0.50
1:B:153:PHE:O	1:B:157:HIS:HD2	1.93	0.50
1:D:40:HIS:O	1:D:52:HIS:HD2	1.95	0.50
1:B:8:ASN:HD22	1:B:10:LEU:H	1.58	0.49
1:D:18:VAL:CG1	1:D:136:THR:HG21	2.42	0.49
1:B:102:LYS:NZ	1:C:160:GLU:OE1	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:LEU:HD11	1:E:51:VAL:HG12	1.95	0.49
1:E:8:ASN:HD22	1:E:8:ASN:C	2.22	0.47
1:C:18:VAL:CG1	1:C:136:THR:HG21	2.45	0.47
1:C:94:LYS:NZ	1:C:116:GLU:OE2	2.48	0.47
1:B:8:ASN:HD22	1:B:8:ASN:C	2.23	0.47
1:B:18:VAL:HG13	1:B:136:THR:HG21	1.97	0.46
1:B:47:GLN:HG2	1:B:47:GLN:O	2.16	0.46
1:E:4:HIS:CE1	1:F:44:LYS:HE3	2.50	0.46
1:E:8:ASN:HD22	1:E:10:LEU:H	1.62	0.46
1:F:71:GLU:O	1:F:74:VAL:HG22	2.16	0.46
1:E:43:LEU:HD11	1:E:51:VAL:CG1	2.46	0.45
1:D:8:ASN:HD22	1:D:10:LEU:H	1.64	0.45
1:A:94:LYS:H	1:A:94:LYS:CD	2.29	0.44
1:C:94:LYS:N	1:C:94:LYS:CD	2.81	0.43
1:F:8:ASN:ND2	1:F:10:LEU:H	2.16	0.43
1:B:8:ASN:ND2	1:B:10:LEU:H	2.15	0.43
1:D:13:ASN:HD22	1:D:14:ALA:H	1.64	0.43
1:E:18:VAL:CG1	1:E:136:THR:HG21	2.48	0.43
1:C:94:LYS:HE2	1:C:112:GLU:OE1	2.18	0.43
1:A:94:LYS:CE	1:A:116:GLU:OE2	2.67	0.43
1:F:18:VAL:CG1	1:F:136:THR:HG21	2.49	0.43
1:A:18:VAL:CG1	1:A:136:THR:HG21	2.49	0.43
1:F:8:ASN:HD22	1:F:8:ASN:C	2.27	0.43
1:A:85:GLN:H	1:A:85:GLN:NE2	2.16	0.43
1:B:85:GLN:NE2	1:B:85:GLN:H	2.16	0.43
1:A:8:ASN:HD22	1:A:10:LEU:H	1.67	0.42
1:A:94:LYS:HD2	1:A:113:ARG:CZ	2.49	0.42
1:C:43:LEU:H	1:C:43:LEU:HD12	1.83	0.42
1:E:43:LEU:HD13	1:E:103:ILE:HG12	2.01	0.42
1:D:85:GLN:NE2	1:D:85:GLN:H	2.17	0.42
1:C:40:HIS:CE1	1:C:52:HIS:CE1	3.07	0.42
1:D:8:ASN:ND2	1:D:10:LEU:H	2.18	0.41
1:A:18:VAL:HG13	1:A:136:THR:HG21	2.01	0.41
1:E:40:HIS:CE1	1:E:52:HIS:CE1	3.08	0.41
1:E:8:ASN:ND2	1:E:10:LEU:H	2.18	0.41
1:D:43:LEU:HD12	1:D:43:LEU:N	2.34	0.41
1:F:85:GLN:H	1:F:85:GLN:NE2	2.18	0.41
1:F:40:HIS:CE1	1:F:52:HIS:CE1	3.09	0.41
1:C:8:ASN:HD22	1:C:10:LEU:H	1.69	0.41
1:F:43:LEU:H	1:F:43:LEU:HD12	1.86	0.41
1:E:85:GLN:H	1:E:85:GLN:NE2	2.19	0.40

All (1) 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)
5:C:2046:HOH:O	5:C:2046:HOH:O[2_665]	1.34	0.86

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	161/162 (99%)	158 (98%)	3 (2%)	0	100	100
1	B	161/162 (99%)	160 (99%)	1 (1%)	0	100	100
1	C	158/162 (98%)	156 (99%)	2 (1%)	0	100	100
1	D	159/162 (98%)	157 (99%)	2 (1%)	0	100	100
1	E	161/162 (99%)	160 (99%)	1 (1%)	0	100	100
1	F	161/162 (99%)	160 (99%)	1 (1%)	0	100	100
All	All	961/972 (99%)	951 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	138/137 (101%)	135 (98%)	3 (2%)	45	13
1	B	138/137 (101%)	135 (98%)	3 (2%)	45	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	135/137 (98%)	132 (98%)	3 (2%)	45	13
1	D	136/137 (99%)	130 (96%)	6 (4%)	25	2
1	E	138/137 (101%)	137 (99%)	1 (1%)	76	54
1	F	138/137 (101%)	134 (97%)	4 (3%)	37	7
All	All	823/822 (100%)	803 (98%)	20 (2%)	43	12

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	85	GLN
1	A	94	LYS
1	B	8	ASN
1	B	94	LYS
1	B	161	LYS
1	C	8	ASN
1	C	43	LEU
1	C	94	LYS
1	D	8	ASN
1	D	13	ASN
1	D	43	LEU
1	D	85	GLN
1	D	94	LYS
1	D	162	SER
1	E	8	ASN
1	F	1	MET
1	F	8	ASN
1	F	35	VAL
1	F	43	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	GLN
1	A	85	GLN
1	B	8	ASN
1	B	38	GLN
1	B	47	GLN
1	B	85	GLN

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Mol	Chain	Res	Type
1	B	157	HIS
1	C	8	ASN
1	C	38	GLN
1	C	85	GLN
1	D	8	ASN
1	D	13	ASN
1	D	38	GLN
1	D	52	HIS
1	D	85	GLN
1	E	8	ASN
1	E	38	GLN
1	E	85	GLN
1	F	8	ASN
1	F	38	GLN
1	F	85	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TRS	E	1164	-	7,7,7	1.31	1 (14%)	9,9,9	1.04	0
3	TRS	B	1164	-	7,7,7	1.13	1 (14%)	9,9,9	0.73	0
4	EDO	D	1164	-	3,3,3	2.50	1 (33%)	2,2,2	0.86	0

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
3	TRS	E	1164	-	-	0/9/9/9	-
3	TRS	B	1164	-	-	0/9/9/9	-
4	EDO	D	1164	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1164	EDO	O1-C1	3.81	1.61	1.42
3	E	1164	TRS	C3-C	-3.10	1.44	1.53
3	B	1164	TRS	C3-C	-2.73	1.45	1.53

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	162/162 (100%)	-0.21	3 (1%) 66 68	11, 16, 25, 44	1 (0%)
1	B	162/162 (100%)	-0.13	4 (2%) 58 60	11, 16, 25, 43	1 (0%)
1	C	159/162 (98%)	-0.19	6 (3%) 44 47	11, 16, 24, 39	1 (0%)
1	D	160/162 (98%)	-0.14	5 (3%) 51 54	11, 16, 25, 50	1 (0%)
1	E	162/162 (100%)	-0.15	6 (3%) 45 48	11, 16, 25, 49	1 (0%)
1	F	162/162 (100%)	-0.16	5 (3%) 51 54	11, 16, 24, 49	1 (0%)
All	All	967/972 (99%)	-0.16	29 (2%) 52 55	11, 16, 25, 50	6 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	3	THR	6.6
1	D	4	HIS	5.3
1	B	3	THR	5.0
1	C	162	SER	4.8
1	F	3	THR	4.7
1	D	162	SER	4.6
1	F	1	MET	4.3
1	A	1	MET	4.2
1	F	4	HIS	4.1
1	E	1	MET	4.0
1	E	3	THR	3.9
1	D	5	LYS	3.8
1	B	47	GLN	3.8
1	E	2	LYS	3.3
1	B	1	MET	3.2
1	B	2	LYS	3.2
1	E	4	HIS	3.2
1	D	161	LYS	2.9
1	C	4	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	94	LYS	2.7
1	F	130	GLU	2.6
1	C	161	LYS	2.6
1	F	2	LYS	2.5
1	A	3	THR	2.5
1	E	43	LEU	2.4
1	C	5	LYS	2.4
1	E	5	LYS	2.4
1	C	13	ASN	2.2
1	C	12	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	A	1163	1/1	0.86	0.18	25,25,25,25	1
2	FE	B	1163	1/1	0.87	0.23	27,27,27,27	1
4	EDO	D	1164	4/4	0.90	0.11	21,22,22,24	0
2	FE	D	1163	1/1	0.91	0.17	29,29,29,29	1
2	FE	F	1163	1/1	0.92	0.15	28,28,28,28	1
2	FE	C	1163	1/1	0.94	0.15	31,31,31,31	1
2	FE	E	1163	1/1	0.95	0.13	27,27,27,27	1
3	TRS	B	1164	8/8	0.97	0.05	14,15,16,16	0
3	TRS	E	1164	8/8	0.98	0.04	14,15,15,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.