



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 AM UTC

PDB ID : 1GRW / pdb_00001grw
Title : C. elegans major sperm protein
Authors : Baker, A.M.E.; Roberts, T.M.; Stewart, M.
Deposited on : 2001-12-18
Resolution : 2.60 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)	:	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

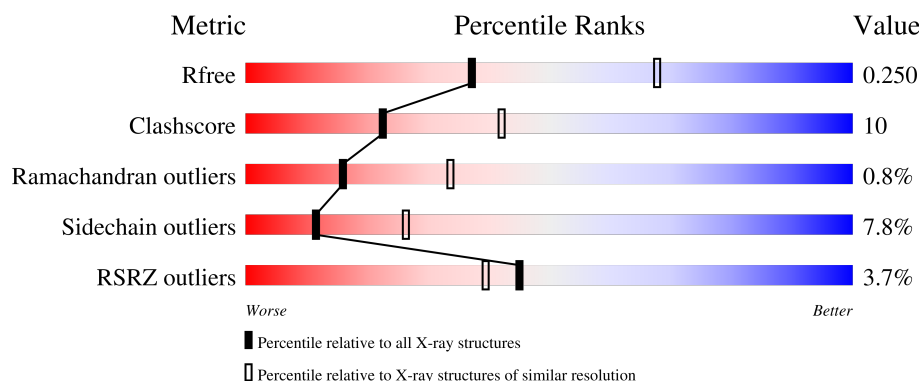
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	126	
1	B	126	
1	C	126	
1	D	126	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3986 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 MAJOR SPERM PROTEIN 31/40/142.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	124	Total	C	N	O	S	36	0	0
			978	614	175	185	4			
1	B	124	Total	C	N	O	S	56	0	0
			978	614	175	185	4			
1	C	124	Total	C	N	O	S	41	0	0
			978	614	175	185	4			
1	D	124	Total	C	N	O	S	34	0	0
			978	614	175	185	4			

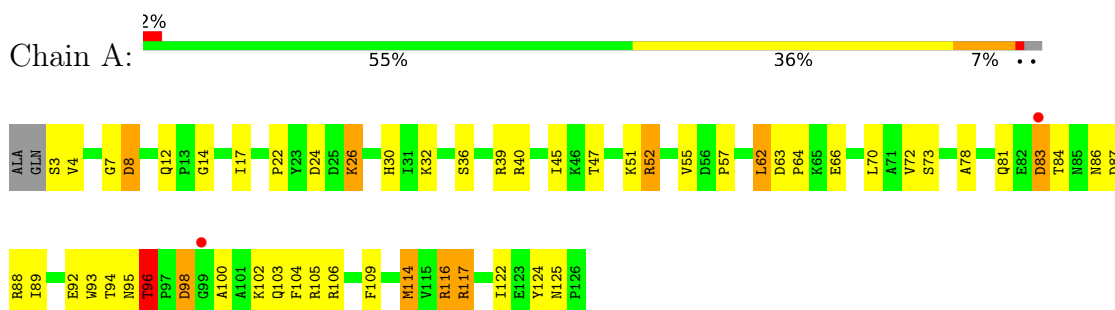
- Molecule 2 is water.

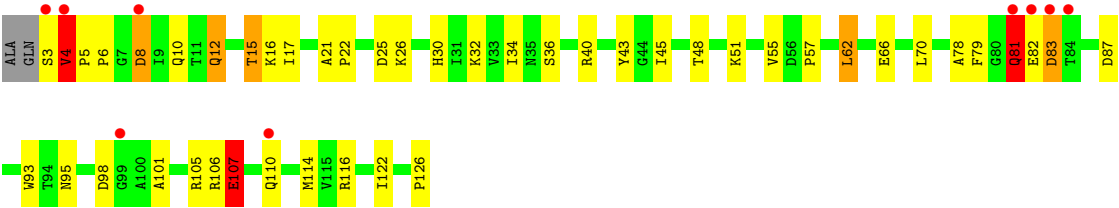
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	27	Total	O	1	1
			27	27		
2	B	14	Total	O	0	0
			14	14		
2	C	15	Total	O	0	0
			15	15		
2	D	18	Total	O	0	0
			18	18		

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 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: MAJOR SPERM PROTEIN 31/40/142





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	53.48Å 53.48Å 457.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.60) 99.3 (20.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.42Å)	Xtriage
Refinement program	REFMAC 4.0.0	Depositor
R, R_{free}	0.228 , 0.256 0.224 , 0.250	Depositor DCC
R_{free} test set	1293 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3986	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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	1.55	6/1002 (0.6%)	2.38	31/1360 (2.3%)
1	B	1.28	10/1002 (1.0%)	2.14	30/1360 (2.2%)
1	C	1.19	7/1002 (0.7%)	2.10	37/1360 (2.7%)
1	D	1.28	5/1002 (0.5%)	1.94	23/1360 (1.7%)
All	All	1.33	28/4008 (0.7%)	2.15	121/5440 (2.2%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	SER	C-N	31.86	1.69	1.33
1	B	39	ARG	CD-NE	-17.38	1.22	1.46
1	D	105	ARG	NE-CZ	-17.17	1.14	1.33
1	D	82	GLU	CB-CG	15.08	1.97	1.52
1	C	117	ARG	CB-CG	-14.98	1.07	1.52
1	A	39	ARG	CZ-NH1	12.30	1.50	1.32
1	B	3	SER	C-N	-12.12	1.19	1.33
1	C	39	ARG	CG-CD	-11.71	1.17	1.52
1	B	92	GLU	CG-CD	-11.20	1.24	1.52
1	A	3	SER	CA-C	10.26	1.74	1.52
1	A	88	ARG	NE-CZ	-10.24	1.21	1.33
1	C	3	SER	C-N	9.38	1.44	1.33
1	A	39	ARG	CZ-NH2	-9.26	1.21	1.33
1	D	106	ARG	CB-CG	-8.46	1.27	1.52
1	C	83	ASP	CB-CG	-7.74	1.32	1.52
1	B	51	LYS	CB-CG	7.55	1.75	1.52
1	D	51	LYS	CB-CG	7.55	1.75	1.52
1	B	126	PRO	N-CD	7.26	1.57	1.47
1	C	50	MET	CB-CG	-6.72	1.32	1.52
1	C	46	LYS	CB-CG	6.61	1.72	1.52
1	C	126	PRO	N-CD	5.96	1.56	1.47
1	B	81	GLN	CB-CG	-5.56	1.35	1.52
1	B	3	SER	CA-C	5.49	1.64	1.52
1	B	107	GLU	CB-CG	-5.40	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	126	PRO	N-CD	5.40	1.55	1.47
1	A	83	ASP	CB-CG	5.38	1.65	1.52
1	B	75	ASP	CB-CG	-5.19	1.39	1.52
1	B	110	GLN	CB-CG	5.09	1.67	1.52

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	SER	CA-C-N	27.14	172.34	122.13
1	A	3	SER	C-N-CA	27.14	172.34	122.13
1	A	3	SER	O-C-N	-25.61	82.03	123.00
1	B	3	SER	CA-C-N	24.68	167.78	122.13
1	B	3	SER	C-N-CA	24.68	167.78	122.13
1	C	3	SER	CA-C-N	-19.10	86.80	122.13
1	C	3	SER	C-N-CA	-19.10	86.80	122.13
1	B	3	SER	O-C-N	-18.75	92.99	123.00
1	C	117	ARG	CA-CB-CG	17.34	148.78	114.10
1	D	83	ASP	CA-CB-CG	14.54	127.14	112.60
1	D	4	VAL	N-CA-CB	13.37	129.92	111.21
1	D	51	LYS	CA-CB-CG	-13.31	87.48	114.10
1	A	88	ARG	NE-CZ-NH2	-12.98	107.52	119.20
1	A	39	ARG	NE-CZ-NH2	12.08	130.07	119.20
1	A	117	ARG	NE-CZ-NH1	11.14	132.65	121.50
1	A	83	ASP	CA-CB-CG	-10.94	101.66	112.60
1	A	52	ARG	NE-CZ-NH2	10.72	128.85	119.20
1	A	98	ASP	CA-CB-CG	-10.71	101.89	112.60
1	A	117	ARG	CD-NE-CZ	10.03	138.44	124.40
1	C	3	SER	O-C-N	9.94	138.90	123.00
1	A	88	ARG	NE-CZ-NH1	9.85	131.35	121.50
1	C	10	GLN	OE1-CD-NE2	-9.83	112.77	122.60
1	C	117	ARG	CB-CG-CD	9.23	132.52	111.30
1	B	39	ARG	CG-CD-NE	9.21	132.27	112.00
1	D	4	VAL	CA-C-O	9.13	132.19	119.95
1	A	7	GLY	O-C-N	-9.00	115.07	122.81
1	A	7	GLY	CA-C-O	8.66	131.82	122.47
1	A	88	ARG	CD-NE-CZ	-8.32	112.75	124.40
1	A	39	ARG	NE-CZ-NH1	-7.94	113.56	121.50
1	B	109	PHE	CA-C-O	7.57	127.46	119.14
1	B	125	ASN	CA-C-O	7.52	126.53	119.99
1	C	119	ASN	CA-CB-CG	-7.44	105.16	112.60
1	A	51	LYS	CA-CB-CG	-7.36	99.38	114.10
1	B	92	GLU	CA-CB-CG	7.29	128.68	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	ARG	CA-C-N	7.19	131.23	120.31
1	C	106	ARG	C-N-CA	7.19	131.23	120.31
1	D	79	PHE	CA-CB-CG	-7.11	106.69	113.80
1	C	16	LYS	O-C-N	6.75	129.61	123.26
1	A	117	ARG	NE-CZ-NH2	-6.74	113.13	119.20
1	B	43	TYR	CA-C-N	6.63	126.16	121.65
1	B	43	TYR	C-N-CA	6.63	126.16	121.65
1	C	99	GLY	CA-C-N	6.55	134.06	121.54
1	C	99	GLY	C-N-CA	6.55	134.06	121.54
1	B	14	GLY	N-CA-C	6.50	122.73	114.66
1	A	86	ASN	N-CA-C	6.48	120.50	111.56
1	C	116	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	D	82	GLU	CA-CB-CG	-6.44	101.23	114.10
1	C	114	MET	N-CA-C	6.39	119.31	108.90
1	D	17	ILE	CA-C-N	-6.31	115.37	123.19
1	D	17	ILE	C-N-CA	-6.31	115.37	123.19
1	D	81	GLN	N-CA-C	6.28	124.17	110.80
1	B	116	ARG	NE-CZ-NH1	-6.26	115.24	121.50
1	D	107	GLU	CB-CG-CD	6.12	123.00	112.60
1	A	52	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	C	103	GLN	OE1-CD-NE2	6.09	128.69	122.60
1	B	99	GLY	N-CA-C	-6.08	104.06	111.35
1	D	122	ILE	CB-CA-C	-6.07	103.62	110.96
1	C	88	ARG	NE-CZ-NH1	-6.06	115.44	121.50
1	A	14	GLY	N-CA-C	6.04	122.15	114.66
1	B	84	THR	N-CA-CB	-6.00	102.32	110.95
1	B	20	ASN	CA-CB-CG	5.90	118.50	112.60
1	C	122	ILE	N-CA-CB	5.89	117.71	111.00
1	B	92	GLU	CB-CG-CD	5.88	122.59	112.60
1	C	17	ILE	CA-C-N	-5.85	115.94	123.19
1	C	17	ILE	C-N-CA	-5.85	115.94	123.19
1	A	116	ARG	NE-CZ-NH1	-5.82	115.68	121.50
1	C	113	GLY	N-CA-C	5.81	118.27	110.43
1	A	103	GLN	CA-C-O	5.78	128.03	120.11
1	B	79	PHE	N-CA-C	5.72	118.00	111.02
1	B	86	ASN	N-CA-C	5.70	119.91	111.87
1	C	16	LYS	CA-C-O	-5.66	114.92	121.26
1	B	105	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	D	101	ALA	O-C-N	5.57	129.11	122.20
1	D	15	THR	N-CA-CB	-5.56	103.61	111.00
1	A	100	ALA	N-CA-C	-5.51	100.90	109.72
1	D	40	ARG	NH1-CZ-NH2	5.49	126.43	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ILE	CA-CB-CG1	5.46	119.68	110.40
1	B	95	ASN	CA-C-O	-5.45	114.55	120.81
1	A	105	ARG	NE-CZ-NH2	5.43	124.09	119.20
1	B	42	GLY	CA-C-N	-5.39	113.75	122.81
1	B	42	GLY	C-N-CA	-5.39	113.75	122.81
1	C	58	PRO	CA-C-O	5.39	125.70	118.90
1	A	104	PHE	N-CA-C	5.39	118.14	110.10
1	C	122	ILE	CB-CA-C	-5.37	104.46	110.96
1	D	51	LYS	CB-CG-CD	-5.36	98.98	111.30
1	C	26	LYS	CA-C-N	-5.35	114.92	122.94
1	C	26	LYS	C-N-CA	-5.35	114.92	122.94
1	B	106	ARG	NE-CZ-NH2	5.34	124.01	119.20
1	D	105	ARG	CD-NE-CZ	-5.33	116.94	124.40
1	C	119	ASN	O-C-N	5.32	129.34	123.16
1	B	92	GLU	CA-C-N	-5.32	113.60	122.21
1	B	92	GLU	C-N-CA	-5.32	113.60	122.21
1	D	12	GLN	OE1-CD-NE2	-5.32	117.28	122.60
1	B	3	SER	N-CA-C	-5.31	96.13	111.00
1	B	7	GLY	O-C-N	-5.30	117.13	122.59
1	C	85	ASN	CA-C-N	-5.28	114.01	122.62
1	C	85	ASN	C-N-CA	-5.28	114.01	122.62
1	C	119	ASN	CA-C-O	-5.25	114.88	120.92
1	B	20	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	D	95	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	81	GLN	CA-C-O	-5.20	113.15	119.03
1	A	78	ALA	CA-C-O	5.18	127.19	121.39
1	C	83	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	106	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	C	56	ASP	CB-CA-C	-5.14	103.33	110.16
1	C	116	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	125	ASN	CA-C-O	5.10	125.64	120.38
1	C	125	ASN	CA-C-O	5.10	125.08	120.09
1	A	96	THR	N-CA-CB	-5.08	101.73	110.01
1	C	18	VAL	CA-C-O	-5.08	115.10	120.48
1	D	25	ASP	N-CA-CB	-5.04	102.79	111.21
1	D	66	GLU	CA-C-N	-5.04	114.67	122.59
1	D	66	GLU	C-N-CA	-5.04	114.67	122.59
1	D	95	ASN	CA-CB-CG	-5.04	107.56	112.60
1	C	88	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	C	10	GLN	CG-CD-NE2	5.03	123.94	116.40
1	D	26	LYS	CA-C-O	-5.03	115.69	120.92
1	C	52	ARG	NE-CZ-NH1	-5.02	116.48	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ALA	CA-C-N	-5.02	114.94	122.81
1	B	38	ALA	C-N-CA	-5.02	114.94	122.81
1	A	81	GLN	O-C-N	5.00	127.69	122.23

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	978	0	955	26	4
1	B	978	0	954	18	0
1	C	978	0	955	18	0
1	D	978	0	955	17	4
2	A	27	0	0	2	0
2	B	14	0	0	0	0
2	C	15	0	0	0	0
2	D	18	0	0	1	0
All	All	3986	0	3819	77	4

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 (77) 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:40:ARG:HD2	1:A:96:THR:HG21	1.55	0.88
1:C:105:ARG:HB3	1:C:107:GLU:OE1	1.75	0.87
1:A:26:LYS:O	2:A:2006:HOH:O	1.94	0.85
1:D:45:ILE:HG21	1:D:55:VAL:HG11	1.65	0.78
1:B:88:ARG:HH22	1:C:110:GLN:HB3	1.54	0.72
1:B:57:PRO:HD2	1:B:70:LEU:HD23	1.72	0.70
1:B:4:VAL:HG23	1:B:5:PRO:HD2	1.74	0.69
1:A:93:TRP:CZ2	1:A:116:ARG:HD3	2.28	0.68
1:A:72:VAL:HG11	1:A:89:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLN:OE1	1:A:32:LYS:HD3	1.95	0.66
1:C:21:ALA:HB1	1:C:22:PRO:HA	1.77	0.66
1:B:45:ILE:HG21	1:B:55:VAL:HG11	1.76	0.65
1:D:93:TRP:CZ2	1:D:116:ARG:HD3	2.33	0.64
1:A:52:ARG:NH1	1:A:87:ASP:OD2	2.31	0.63
1:B:72:VAL:HG11	1:B:89:ILE:HD11	1.80	0.63
1:A:57:PRO:HD2	1:A:70:LEU:HD23	1.82	0.62
1:A:94:THR:HG22	1:A:109:PHE:HE1	1.65	0.61
1:B:94:THR:HG22	1:B:109:PHE:HE1	1.64	0.61
1:A:84:THR:HB	1:A:124:TYR:CD2	2.35	0.61
1:B:94:THR:HG22	1:B:109:PHE:CE1	2.37	0.60
1:A:40:ARG:CD	1:A:96:THR:HG21	2.32	0.56
1:C:94:THR:HG22	1:C:109:PHE:HE1	1.71	0.56
1:B:84:THR:HG23	1:B:124:TYR:CD2	2.41	0.55
1:A:45:ILE:HG21	1:A:55:VAL:HG11	1.88	0.54
1:D:5:PRO:HB3	1:D:114:MET:HE1	1.88	0.54
1:D:48:THR:OG1	1:D:87:ASP:HA	2.08	0.53
1:D:8:ASP:OD2	1:D:8:ASP:N	2.42	0.53
1:A:22:PRO:HB2	1:A:24:ASP:OD1	2.09	0.52
1:A:63:ASP:HB3	1:A:64:PRO:HD2	1.90	0.52
1:C:57:PRO:HD2	1:C:70:LEU:HD23	1.90	0.52
1:D:10:GLN:HG2	1:D:34:ILE:HD12	1.90	0.52
1:D:21:ALA:HB1	1:D:22:PRO:HA	1.91	0.52
1:B:93:TRP:CZ2	1:B:116:ARG:HD3	2.45	0.51
1:A:89:ILE:CD1	1:A:122:ILE:HD11	2.39	0.51
1:C:72:VAL:HG11	1:C:89:ILE:HD11	1.92	0.51
1:D:78:ALA:HB3	1:D:81:GLN:HB2	1.92	0.51
1:D:107:GLU:HA	1:D:110:GLN:NE2	2.26	0.51
1:C:107:GLU:CD	1:C:107:GLU:H	2.18	0.50
1:C:48:THR:OG1	1:C:87:ASP:HA	2.12	0.49
1:D:3:SER:OG	1:D:4:VAL:N	2.38	0.49
1:A:8:ASP:HB3	2:A:2002:HOH:O	2.13	0.49
1:C:15:THR:HB	2:D:2018:HOH:O	2.12	0.49
1:B:30:HIS:HA	1:B:70:LEU:O	2.12	0.48
1:C:94:THR:HG22	1:C:109:PHE:CE1	2.49	0.48
1:A:62:LEU:HD12	1:A:66:GLU:HG2	1.96	0.48
1:A:92:GLU:OE2	1:A:117:ARG:NH2	2.46	0.47
1:C:93:TRP:CZ2	1:C:116:ARG:HD3	2.49	0.47
1:C:62:LEU:HD11	1:C:68:VAL:HB	1.97	0.47
1:C:25:ASP:HB2	1:C:27:HIS:CE1	2.50	0.47
1:B:5:PRO:HB3	1:B:114:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:PRO:HG2	1:D:116:ARG:HB2	1.99	0.46
1:D:12:GLN:OE1	1:D:32:LYS:HD3	2.16	0.45
1:A:94:THR:HG22	1:A:109:PHE:CE1	2.47	0.45
1:A:17:ILE:CG2	1:A:122:ILE:HD13	2.47	0.44
1:C:63:ASP:HB3	1:C:64:PRO:HD2	1.99	0.44
1:D:43:TYR:CD2	1:D:62:LEU:HD22	2.52	0.43
1:D:15:THR:O	1:D:16:LYS:HB3	2.17	0.43
1:A:8:ASP:OD1	1:A:8:ASP:N	2.52	0.43
1:C:6:PRO:HG2	1:C:116:ARG:HB2	2.01	0.43
1:B:43:TYR:CD2	1:B:62:LEU:HD22	2.55	0.42
1:B:48:THR:OG1	1:B:87:ASP:HA	2.19	0.42
1:B:25:ASP:O	1:B:27:HIS:CD2	2.73	0.42
1:A:52:ARG:HH11	1:A:52:ARG:HD2	1.62	0.42
1:A:4:VAL:HG23	1:A:95:ASN:HD22	1.85	0.41
1:A:30:HIS:HA	1:A:70:LEU:O	2.20	0.41
1:D:30:HIS:HA	1:D:70:LEU:O	2.21	0.41
1:B:21:ALA:HB2	1:B:126:PRO:HA	2.02	0.41
1:D:114:MET:HB3	1:D:114:MET:HE2	1.78	0.41
1:A:102:LYS:HG2	1:A:102:LYS:O	2.20	0.40
1:A:63:ASP:HB3	1:A:64:PRO:CD	2.52	0.40
1:B:48:THR:HG21	1:B:88:ARG:HG2	2.03	0.40
1:D:57:PRO:HD2	1:D:70:LEU:HD23	2.03	0.40
1:C:114:MET:HE3	1:C:114:MET:HB2	1.91	0.40
1:A:114:MET:HE3	1:A:114:MET:HB2	1.79	0.40
1:C:45:ILE:HG21	1:C:55:VAL:HG11	2.03	0.40
1:B:72:VAL:HG11	1:B:89:ILE:CD1	2.48	0.40
1:B:88:ARG:NH2	1:C:110:GLN:HB3	2.29	0.40

All (4) 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:A:83:ASP:OD2	1:D:98:ASP:OD2[7_545]	1.53	0.67
1:A:83:ASP:OD1	1:D:98:ASP:OD1[7_545]	2.01	0.19
1:A:83:ASP:CG	1:D:98:ASP:OD2[7_545]	2.04	0.16
1:A:83:ASP:OD1	1:D:98:ASP:OD2[7_545]	2.12	0.08

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	122/126 (97%)	118 (97%)	4 (3%)	0	100	100
1	B	122/126 (97%)	114 (93%)	6 (5%)	2 (2%)	7	16
1	C	122/126 (97%)	118 (97%)	3 (2%)	1 (1%)	16	34
1	D	122/126 (97%)	117 (96%)	4 (3%)	1 (1%)	16	34
All	All	488/504 (97%)	467 (96%)	17 (4%)	4 (1%)	16	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	ALA
1	C	100	ALA
1	B	4	VAL
1	D	81	GLN

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	106/107 (99%)	97 (92%)	9 (8%)	10	22
1	B	106/107 (99%)	94 (89%)	12 (11%)	5	12
1	C	106/107 (99%)	100 (94%)	6 (6%)	18	40
1	D	106/107 (99%)	100 (94%)	6 (6%)	18	40
All	All	424/428 (99%)	391 (92%)	33 (8%)	11	26

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	26	LYS
1	A	36	SER
1	A	47	THR
1	A	62	LEU
1	A	73	SER
1	A	96	THR
1	A	98	ASP
1	A	114	MET
1	B	4	VAL
1	B	8	ASP
1	B	24	ASP
1	B	36	SER
1	B	62	LEU
1	B	65	LYS
1	B	84	THR
1	B	98	ASP
1	B	102	LYS
1	B	103	GLN
1	B	105	ARG
1	B	117	ARG
1	C	4	VAL
1	C	24	ASP
1	C	36	SER
1	C	62	LEU
1	C	114	MET
1	C	117	ARG
1	D	4	VAL
1	D	8	ASP
1	D	36	SER
1	D	62	LEU
1	D	83	ASP
1	D	107	GLU

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	30	HIS
1	A	49	ASN
1	B	27	HIS
1	B	49	ASN

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Mol	Chain	Res	Type
1	C	27	HIS
1	C	49	ASN
1	C	110	GLN
1	D	110	GLN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	3:SER	C	4:VAL	N	1.69
1	B	3:SER	C	4:VAL	N	1.19

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	123/126 (97%)	-0.04	2 (1%) 70 66	27, 45, 66, 88	8 (6%)
1	B	123/126 (97%)	0.10	5 (4%) 41 36	30, 49, 78, 88	12 (9%)
1	C	123/126 (97%)	-0.00	2 (1%) 70 66	19, 48, 75, 90	9 (7%)
1	D	124/126 (98%)	0.06	9 (7%) 21 17	26, 46, 71, 93	10 (8%)
All	All	493/504 (97%)	0.03	18 (3%) 45 39	19, 47, 75, 93	39 (7%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	84	THR	4.0
1	A	83	ASP	3.6
1	D	83	ASP	3.1
1	A	99	GLY	3.0
1	B	99	GLY	2.8
1	C	83	ASP	2.7
1	D	3	SER	2.7
1	C	86	ASN	2.6
1	D	82	GLU	2.5
1	D	110	GLN	2.4
1	D	81	GLN	2.4
1	D	99	GLY	2.3
1	B	4	VAL	2.3
1	B	81	GLN	2.2
1	D	8	ASP	2.2
1	B	108	TRP	2.1
1	B	101	ALA	2.0
1	D	4	VAL	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.