



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:20 PM UTC

PDB ID : 9C2Y / pdb_00009c2y
Title : Crystal Structure of JF1cpCasp2 in complex with MUR-65
Authors : Fuller, J.L.; Finzel, B.C.; Shi, K.
Deposited on : 2024-05-31
Resolution : 1.96 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

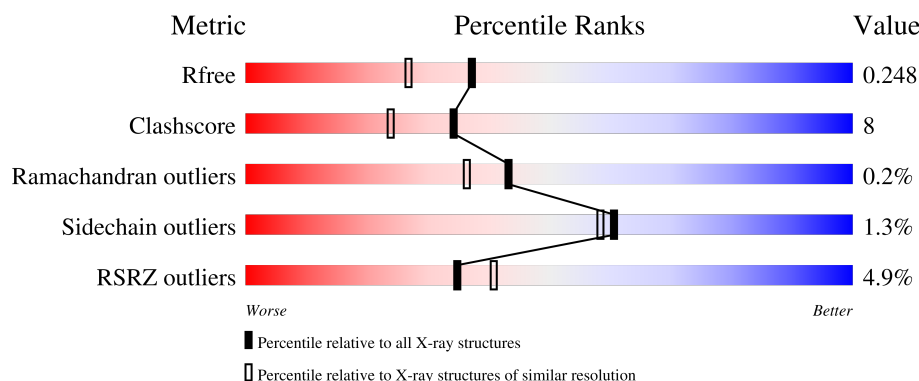
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	282	5% 69% 15% 16%
1	B	282	4% 77% 12% 11%
1	C	282	4% 70% 14% 16%
1	D	282	2% 74% 10% 16%
2	F	5	20% 20% 40% 40%

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Mol	Chain	Length	Quality of chain
2	G	5	
2	H	5	
2	I	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	A1AT7	F	4	-	X	-	-
2	ASJ	G	5	-	-	X	-
2	A1AT6	H	1	-	X	-	-
2	A1AT7	H	4	-	X	-	-
2	A1AT7	I	4	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7701 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 JF1cpCasp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	2	0
			1833	1152	326	337	18			
1	B	252	Total	C	N	O	S	0	2	0
			1952	1230	345	357	20			
1	C	238	Total	C	N	O	S	0	2	0
			1849	1161	327	342	19			
1	D	237	Total	C	N	O	S	0	3	0
			1840	1157	327	337	19			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P42575
A	2	HIS	-	expression tag	UNP P42575
A	3	HIS	-	expression tag	UNP P42575
A	4	HIS	-	expression tag	UNP P42575
A	5	HIS	-	expression tag	UNP P42575
A	6	HIS	-	expression tag	UNP P42575
A	7	HIS	-	expression tag	UNP P42575
A	21	ALA	ASP	conflict	UNP P42575
A	123	GLY	-	linker	UNP P42575
A	124	GLY	-	linker	UNP P42575
A	125	VAL	-	linker	UNP P42575
B	1	MET	-	initiating methionine	UNP P42575
B	2	HIS	-	expression tag	UNP P42575
B	3	HIS	-	expression tag	UNP P42575
B	4	HIS	-	expression tag	UNP P42575
B	5	HIS	-	expression tag	UNP P42575
B	6	HIS	-	expression tag	UNP P42575
B	7	HIS	-	expression tag	UNP P42575
B	21	ALA	ASP	conflict	UNP P42575
B	123	GLY	-	linker	UNP P42575
B	124	GLY	-	linker	UNP P42575

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Chain	Residue	Modelled	Actual	Comment	Reference
B	125	VAL	-	linker	UNP P42575
C	1	MET	-	initiating methionine	UNP P42575
C	2	HIS	-	expression tag	UNP P42575
C	3	HIS	-	expression tag	UNP P42575
C	4	HIS	-	expression tag	UNP P42575
C	5	HIS	-	expression tag	UNP P42575
C	6	HIS	-	expression tag	UNP P42575
C	7	HIS	-	expression tag	UNP P42575
C	21	ALA	ASP	conflict	UNP P42575
C	123	GLY	-	linker	UNP P42575
C	124	GLY	-	linker	UNP P42575
C	125	VAL	-	linker	UNP P42575
D	1	MET	-	initiating methionine	UNP P42575
D	2	HIS	-	expression tag	UNP P42575
D	3	HIS	-	expression tag	UNP P42575
D	4	HIS	-	expression tag	UNP P42575
D	5	HIS	-	expression tag	UNP P42575
D	6	HIS	-	expression tag	UNP P42575
D	7	HIS	-	expression tag	UNP P42575
D	21	ALA	ASP	conflict	UNP P42575
D	123	GLY	-	linker	UNP P42575
D	124	GLY	-	linker	UNP P42575
D	125	VAL	-	linker	UNP P42575

- Molecule 2 is a protein called MUR-65.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	F	5	Total C N O 49 35 5 9	0	0	0
2	G	5	Total C N O 49 35 5 9	0	0	0
2	H	5	Total C N O 49 35 5 9	0	0	0
2	I	5	Total C N O 49 35 5 9	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	10	Total O 10 10	0	0

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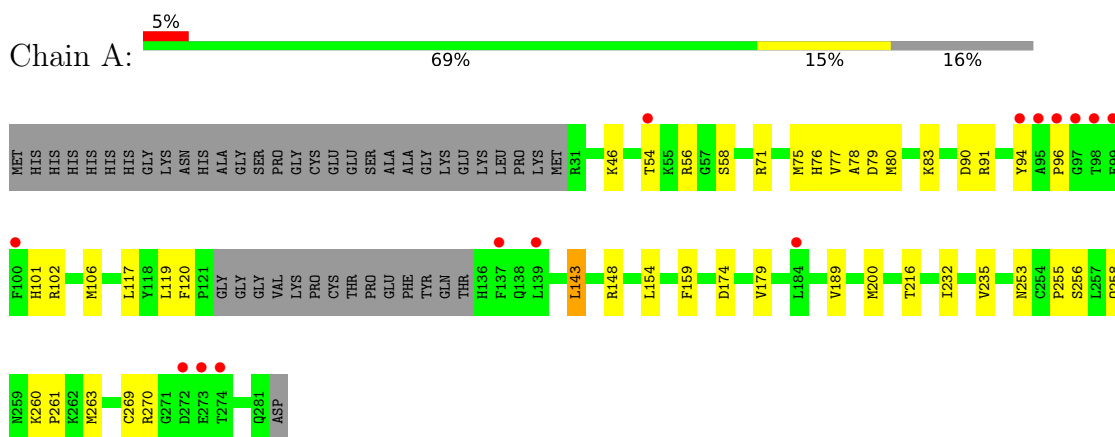
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	6	Total	O	0	0
			6	6		
3	D	8	Total	O	0	0
			8	8		

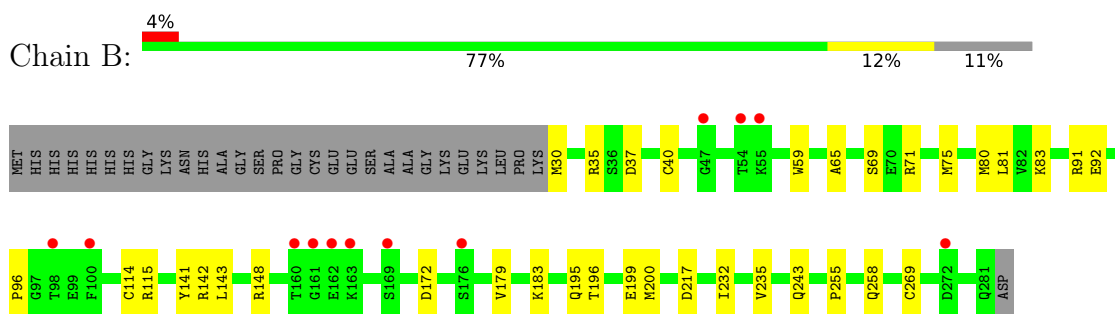
3 Residue-property plots [i](#)

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.

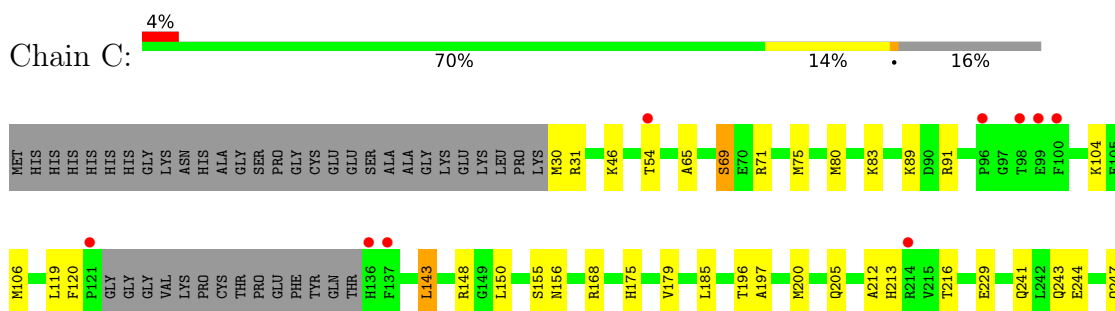
- Molecule 1: JF1cpCasp2

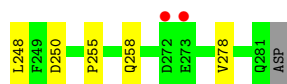


- Molecule 1: JF1cpCasp2

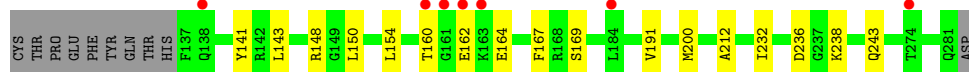
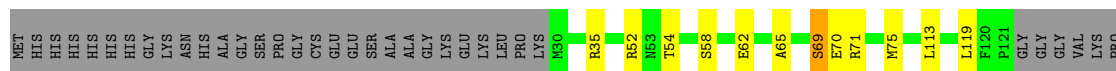
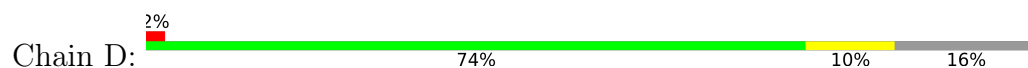


- Molecule 1: JF1cpCasp2

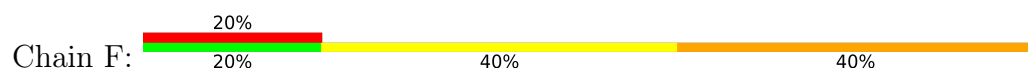




- Molecule 1: JF1cpCasp2



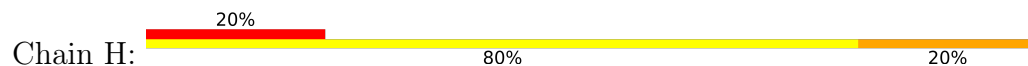
- Molecule 2: MUR-65



- Molecule 2: MUR-65



- Molecule 2: MUR-65



- Molecule 2: MUR-65



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.29Å 130.25Å 78.30Å 90.00° 104.56° 90.00°	Depositor
Resolution (Å)	34.04 – 1.96 34.04 – 1.96	Depositor EDS
% Data completeness (in resolution range)	46.6 (34.04-1.96) 43.3 (34.04-1.96)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.248 0.197 , 0.248	Depositor DCC
R_{free} test set	1943 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7701	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ASJ, A1AT7, A1AT6, UN1

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	0.43	0/1868	0.65	0/2525
1	B	0.45	0/1993	0.67	0/2695
1	C	0.44	0/1884	0.65	0/2545
1	D	0.43	0/1874	0.64	0/2532
2	F	0.86	0/6	2.26	0/7
2	G	1.09	0/6	2.42	0/7
2	H	0.93	0/6	2.90	1/7 (14.3%)
2	I	1.09	0/6	1.23	0/7
All	All	0.44	0/7643	0.66	1/10325 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	3	VAL	CB-CA-C	5.03	120.96	111.40

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	1833	0	1762	34	0
1	B	1952	0	1881	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1849	0	1779	28	0
1	D	1840	0	1777	19	0
2	F	49	0	18	3	0
2	G	49	0	19	7	0
2	H	49	0	18	1	0
2	I	49	0	17	0	0
3	A	7	0	0	0	0
3	B	10	0	0	1	0
3	C	6	0	0	0	0
3	D	8	0	0	0	0
All	All	7701	0	7271	113	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 8.

All (113) 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:B:269:CYS:SG	2:G:5:ASJ:H	1.34	1.64
1:A:269:CYS:SG	2:F:5:ASJ:C	2.03	1.46
1:B:269:CYS:SG	2:G:5:ASJ:C	2.06	1.41
1:B:269:CYS:HG	2:G:5:ASJ:C	1.64	0.96
1:B:35:ARG:HH22	1:B:243:GLN:HE21	1.14	0.90
1:B:75:MET:HE1	1:B:83:LYS:HD2	1.59	0.83
1:B:269:CYS:SG	2:G:5:ASJ:O	2.38	0.81
1:A:256[A]:SER:O	1:A:260:LYS:NZ	2.13	0.81
1:A:75:MET:HE1	1:A:83:LYS:HG3	1.66	0.77
1:C:75:MET:HE1	1:C:83:LYS:HD2	1.68	0.76
1:A:256[B]:SER:O	1:A:260:LYS:NZ	2.21	0.73
1:A:269:CYS:SG	2:F:5:ASJ:HA	2.23	0.73
1:A:120:PHE:O	1:A:148:ARG:NH1	2.22	0.72
1:D:200:MET:HE1	1:D:232:ILE:HD11	1.72	0.72
1:B:35:ARG:NH2	1:B:243:GLN:HE21	1.88	0.71
1:C:241:GLN:HB2	1:C:244:GLU:HG3	1.71	0.70
1:D:200:MET:HE1	1:D:232:ILE:CD1	2.22	0.69
1:A:46:LYS:H	1:A:46:LYS:HD2	1.58	0.69
1:B:40[A]:CYS:SG	3:B:310:HOH:O	2.49	0.69
1:D:143:LEU:HD22	1:D:148:ARG:HD2	1.75	0.69
1:A:119:LEU:HD21	1:A:263:MET:HE1	1.73	0.68
1:B:75:MET:HE3	1:B:80:MET:HG2	1.74	0.68
1:C:54:THR:HG23	2:H:1:A1AT6:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD11	1:A:261:PRO:HG3	1.77	0.66
1:B:269:CYS:SG	2:G:5:ASJ:CA	2.83	0.65
1:C:148:ARG:HG2	1:C:148:ARG:HH11	1.63	0.64
1:C:75:MET:HG2	1:C:80:MET:HG2	1.79	0.63
1:D:150:LEU:HD11	1:D:212:ALA:HB3	1.81	0.63
1:B:71:ARG:HB3	1:B:75:MET:HE2	1.80	0.63
1:C:143:LEU:HD23	1:C:148:ARG:HD2	1.79	0.63
1:B:196:THR:OG1	1:B:199:GLU:HG3	1.98	0.62
1:C:243:GLN:O	1:C:247:GLN:HG3	2.01	0.60
1:B:200:MET:HE1	1:B:232:ILE:CD1	2.32	0.60
1:A:179:VAL:HG13	1:A:189:VAL:HG11	1.84	0.59
1:D:71:ARG:HB3	1:D:75:MET:HE3	1.85	0.59
1:A:200:MET:HE1	1:A:232:ILE:HD12	1.85	0.59
1:C:71:ARG:HB3	1:C:75:MET:HE2	1.84	0.58
1:C:196:THR:O	1:C:200:MET:HG3	2.03	0.58
1:D:35:ARG:HH12	1:D:243:GLN:HE22	1.52	0.57
1:B:35:ARG:HH12	1:B:243:GLN:NE2	2.03	0.56
1:A:46:LYS:H	1:A:46:LYS:CD	2.19	0.56
1:D:154:LEU:HD22	1:D:200:MET:HE3	1.87	0.55
1:C:143:LEU:CD2	1:C:148:ARG:HD2	2.36	0.55
1:D:65:ALA:O	1:D:69:SER:OG	2.13	0.55
1:A:54:THR:HG22	2:F:1:A1AT6:O	2.07	0.55
1:B:35:ARG:HH12	1:B:243:GLN:HE22	1.54	0.55
1:B:200:MET:HE1	1:B:232:ILE:HD11	1.90	0.54
1:B:143:LEU:HD22	1:B:148:ARG:HD2	1.88	0.54
1:A:46:LYS:HG3	1:A:270:ARG:NH2	2.24	0.53
1:A:117:LEU:HD21	1:A:263:MET:HE2	1.90	0.53
1:A:56:ARG:HH21	1:A:91:ARG:NH2	2.08	0.52
1:B:142:ARG:NH1	1:B:217:ASP:OD2	2.43	0.52
1:D:54:THR:HG22	1:D:169:SER:OG	2.10	0.51
1:D:236:ASP:OD2	1:D:238:LYS:HG3	2.11	0.51
1:B:269:CYS:HG	2:G:5:ASJ:H	0.68	0.50
1:A:90:ASP:O	1:B:30:MET:HE1	2.11	0.50
1:A:143:LEU:HD22	1:A:148:ARG:HD3	1.94	0.50
1:B:65:ALA:O	1:B:69:SER:HB2	2.12	0.50
1:A:216:THR:O	1:A:260:LYS:HE2	2.12	0.49
1:A:94:TYR:CD1	1:A:96:PRO:HD3	2.47	0.49
1:B:114:CYS:O	1:B:115:ARG:HG3	2.12	0.49
1:C:213:HIS:HA	1:C:216:THR:HG1	1.77	0.49
1:A:119:LEU:HA	1:A:143:LEU:HD13	1.95	0.49
1:C:175:HIS:O	1:C:179:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:MET:HE1	1:B:232:ILE:HD12	1.95	0.48
1:D:160:THR:O	1:D:160:THR:OG1	2.32	0.48
1:C:120:PHE:O	1:C:148:ARG:NH2	2.47	0.48
1:C:46:LYS:HA	1:C:229:GLU:OE1	2.13	0.47
1:B:172:ASP:OD1	1:B:172:ASP:N	2.44	0.47
1:C:213:HIS:HA	1:C:216:THR:OG1	2.14	0.47
1:B:59:TRP:CE3	1:B:91:ARG:HG2	2.49	0.47
1:C:150:LEU:HD11	1:C:212:ALA:HB3	1.96	0.47
1:D:35:ARG:HH22	1:D:243:GLN:NE2	2.13	0.47
1:B:179:VAL:O	1:B:183:LYS:HG3	2.15	0.46
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.59	0.46
1:D:52:ARG:HA	1:D:58:SER:HA	1.98	0.46
1:C:91:ARG:O	1:C:104:LYS:NZ	2.48	0.45
1:A:101:HIS:CD2	1:A:102:ARG:HG3	2.51	0.45
1:A:106:MET:HG2	1:B:35:ARG:O	2.16	0.45
1:D:52:ARG:NH1	1:D:169:SER:O	2.39	0.45
1:A:159:PHE:CD2	1:A:235:VAL:HA	2.52	0.45
1:A:255:PRO:HA	1:A:258:GLN:HG3	1.98	0.45
1:B:255:PRO:HA	1:B:258:GLN:HG3	1.98	0.45
1:C:30:MET:HG3	1:C:31:ARG:H	1.80	0.45
1:D:119:LEU:HA	1:D:143:LEU:HD13	1.99	0.45
1:A:71:ARG:HA	1:A:71:ARG:HD2	1.74	0.44
1:D:200:MET:CE	1:D:232:ILE:HD11	2.46	0.44
1:B:37:ASP:OD1	1:B:141:TYR:OH	2.34	0.44
1:C:119:LEU:HD12	1:C:185:LEU:HD13	1.99	0.44
1:A:77:VAL:HA	1:A:80:MET:HE3	1.99	0.43
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.80	0.43
1:C:197:ALA:HA	1:C:200:MET:HE2	1.99	0.43
1:B:195:GLN:O	1:B:235:VAL:HG22	2.18	0.43
1:C:156:ASN:O	1:C:168:ARG:HD3	2.18	0.43
1:C:71:ARG:HD2	1:C:71:ARG:HA	1.66	0.43
1:B:71:ARG:CB	1:B:75:MET:HE2	2.45	0.43
1:D:70:GLU:HB3	1:D:71:ARG:HG2	2.01	0.43
1:A:58:SER:OG	1:A:174:ASP:OD2	2.32	0.42
1:C:255:PRO:HA	1:C:258:GLN:HG3	2.01	0.42
1:A:75:MET:HE3	1:A:79:ASP:HB3	2.01	0.42
1:C:205:GLN:HG3	1:C:248:LEU:HD22	2.00	0.42
1:A:154:LEU:HD22	1:A:200:MET:HE3	2.01	0.42
1:C:250:ASP:OD1	1:C:250:ASP:C	2.63	0.42
1:B:195:GLN:C	1:B:235:VAL:HG22	2.46	0.41
1:A:76:HIS:CE1	1:A:78:ALA:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ALA:O	1:C:69:SER:OG	2.35	0.41
1:C:89:LYS:HB2	1:C:106:MET:SD	2.60	0.41
1:D:113:LEU:HD22	1:D:141:TYR:CE2	2.56	0.41
1:C:148:ARG:HD3	1:C:148:ARG:HA	1.87	0.41
1:A:94:TYR:CE1	1:A:96:PRO:HD3	2.57	0.40
1:B:96:PRO:HD2	2:G:1:A1AT6:C22	2.52	0.40
1:A:253:ASN:OD1	1:A:253:ASN:N	2.54	0.40
1:D:113:LEU:HA	1:D:113:LEU:HD23	1.82	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	235/282 (83%)	224 (95%)	11 (5%)	0	100	100
1	B	252/282 (89%)	243 (96%)	9 (4%)	0	100	100
1	C	236/282 (84%)	224 (95%)	12 (5%)	0	100	100
1	D	236/282 (84%)	228 (97%)	6 (2%)	2 (1%)	16	8
2	F	1/5 (20%)	1 (100%)	0	0	100	100
2	G	1/5 (20%)	1 (100%)	0	0	100	100
2	H	1/5 (20%)	1 (100%)	0	0	100	100
2	I	1/5 (20%)	1 (100%)	0	0	100	100
All	All	963/1148 (84%)	923 (96%)	38 (4%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	164	GLU
1	D	162	GLU

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	192/238 (81%)	191 (100%)	1 (0%)	81	82
1	B	205/238 (86%)	204 (100%)	1 (0%)	81	82
1	C	195/238 (82%)	191 (98%)	4 (2%)	47	41
1	D	193/238 (81%)	189 (98%)	4 (2%)	47	41
2	F	1/1 (100%)	1 (100%)	0	100	100
2	G	1/1 (100%)	1 (100%)	0	100	100
2	H	1/1 (100%)	1 (100%)	0	100	100
2	I	1/1 (100%)	1 (100%)	0	100	100
All	All	789/956 (82%)	779 (99%)	10 (1%)	61	58

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	LEU
1	B	92	GLU
1	C	69	SER
1	C	143	LEU
1	C	155	SER
1	C	278	VAL
1	D	62	GLU
1	D	69	SER
1	D	167	PHE
1	D	191	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	HIS
1	A	280	GLN
1	B	76	HIS
1	B	116	HIS

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Mol	Chain	Res	Type
1	B	243	GLN
1	B	259	ASN
1	C	116	HIS
1	C	198	GLN
1	C	253	ASN
1	D	158	HIS
1	D	243	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1AT7	F	4	2	14,14,15	7.33	8 (57%)	16,19,21	4.05	11 (68%)
2	ASJ	G	5	2	7,7,7	1.05	0	5,8,8	1.53	1 (20%)
2	A1AT7	G	4	2	14,14,15	7.61	8 (57%)	16,19,21	4.52	8 (50%)
2	A1AT7	I	4	2	14,14,15	7.44	9 (64%)	16,19,21	4.09	10 (62%)
2	ASJ	F	5	2	7,7,7	1.00	0	5,8,8	1.45	1 (20%)
2	A1AT6	I	1	2	11,12,13	6.81	6 (54%)	13,16,18	5.13	9 (69%)
2	ASJ	H	5	2,1	7,7,7	0.87	0	5,8,8	1.50	1 (20%)
2	ASJ	I	5	2,1	7,7,7	0.99	0	5,8,8	1.70	1 (20%)
2	A1AT6	G	1	2	11,12,13	7.00	6 (54%)	13,16,18	5.43	9 (69%)
2	UN1	H	2	2	8,9,10	0.84	0	5,10,12	1.47	1 (20%)
2	UN1	F	2	2	8,9,10	0.89	0	5,10,12	1.56	1 (20%)
2	A1AT6	F	1	2	11,12,13	7.03	6 (54%)	13,16,18	5.26	9 (69%)
2	UN1	I	2	2	8,9,10	0.99	0	5,10,12	1.33	0
2	UN1	G	2	2	8,9,10	0.93	0	5,10,12	1.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1AT6	H	1	2	11,12,13	7.03	6 (54%)	13,16,18	5.00	10 (76%)
2	A1AT7	H	4	2	14,14,15	7.56	9 (64%)	16,19,21	3.94	10 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1AT7	F	4	2	-	0/0/12/14	0/2/2/2
2	ASJ	G	5	2	-	6/6/6/6	-
2	A1AT7	G	4	2	-	0/0/12/14	0/2/2/2
2	A1AT7	I	4	2	-	0/0/12/14	0/2/2/2
2	ASJ	F	5	2	-	2/6/6/6	-
2	A1AT6	I	1	2	-	0/0/10/12	0/2/2/2
2	ASJ	H	5	2,1	-	3/6/6/6	-
2	ASJ	I	5	2,1	-	4/6/6/6	-
2	A1AT6	G	1	2	-	0/0/10/12	0/2/2/2
2	UN1	H	2	2	-	2/7/8/10	-
2	UN1	F	2	2	-	3/7/8/10	-
2	A1AT6	F	1	2	-	0/0/10/12	0/2/2/2
2	UN1	I	2	2	-	5/7/8/10	-
2	UN1	G	2	2	-	0/7/8/10	-
2	A1AT6	H	1	2	-	0/0/10/12	0/2/2/2
2	A1AT7	H	4	2	-	0/0/12/14	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	4	A1AT7	C27-CB	22.92	1.67	1.39
2	H	4	A1AT7	C27-CB	22.63	1.67	1.39
2	I	4	A1AT7	C27-CB	22.52	1.67	1.39
2	F	4	A1AT7	C27-CB	21.82	1.66	1.39
2	G	1	A1AT6	C20-C19	17.83	1.68	1.39
2	F	1	A1AT6	C20-C19	17.76	1.68	1.39
2	H	1	A1AT6	C20-C19	17.43	1.67	1.39
2	I	1	A1AT6	C20-C19	16.86	1.67	1.39
2	G	4	A1AT7	C23-C24	-10.20	1.23	1.39
2	F	4	A1AT7	C23-C24	-9.94	1.23	1.39
2	H	4	A1AT7	C23-C24	-9.80	1.23	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	4	A1AT7	C23-C24	-9.16	1.24	1.39
2	I	1	A1AT6	C19-C18	8.53	1.47	1.39
2	H	1	A1AT6	C22-C23	-8.43	1.24	1.38
2	H	1	A1AT6	C19-C18	8.38	1.47	1.39
2	F	1	A1AT6	C19-C18	8.24	1.47	1.39
2	I	1	A1AT6	C22-C23	-8.23	1.24	1.38
2	G	1	A1AT6	C19-C18	8.16	1.47	1.39
2	F	1	A1AT6	C22-C23	-7.86	1.25	1.38
2	G	1	A1AT6	C22-C23	-7.78	1.25	1.38
2	I	4	A1AT7	C20-CB	7.19	1.48	1.40
2	H	4	A1AT7	C20-CB	7.18	1.48	1.40
2	G	4	A1AT7	C20-CB	7.08	1.48	1.40
2	F	4	A1AT7	C20-CB	6.86	1.48	1.40
2	F	1	A1AT6	C23-C18	6.50	1.50	1.39
2	G	1	A1AT6	C23-C18	6.24	1.49	1.39
2	H	1	A1AT6	C23-C18	6.15	1.49	1.39
2	I	1	A1AT6	C23-C18	5.90	1.49	1.39
2	F	4	A1AT7	C26-C24	-5.86	1.25	1.38
2	H	4	A1AT7	C26-C24	-5.83	1.25	1.38
2	G	4	A1AT7	CB-CA	5.81	1.58	1.51
2	H	1	A1AT6	C22-C21	-5.60	1.25	1.38
2	I	4	A1AT7	C26-C24	-5.56	1.25	1.38
2	I	1	A1AT6	C22-C21	-5.50	1.26	1.38
2	F	1	A1AT6	C22-C21	-5.50	1.26	1.38
2	I	4	A1AT7	C22-N	5.50	1.42	1.34
2	H	4	A1AT7	CB-CA	5.49	1.58	1.51
2	G	4	A1AT7	C26-C24	-5.46	1.25	1.38
2	G	1	A1AT6	C22-C21	-5.42	1.26	1.38
2	H	1	A1AT6	C19-N	5.30	1.48	1.39
2	H	4	A1AT7	C23-C20	5.18	1.49	1.40
2	F	4	A1AT7	C22-N	5.09	1.41	1.34
2	H	4	A1AT7	C22-N	4.86	1.41	1.34
2	F	4	A1AT7	CB-CA	4.86	1.57	1.51
2	I	4	A1AT7	C22-C21	4.84	1.45	1.35
2	I	4	A1AT7	C23-C20	4.83	1.49	1.40
2	F	1	A1AT6	C19-N	4.72	1.47	1.39
2	G	1	A1AT6	C19-N	4.71	1.47	1.39
2	G	4	A1AT7	C23-C20	4.69	1.48	1.40
2	G	4	A1AT7	C22-N	4.56	1.41	1.34
2	G	4	A1AT7	C22-C21	4.55	1.45	1.35
2	F	4	A1AT7	C23-C20	4.50	1.48	1.40
2	H	4	A1AT7	C22-C21	4.43	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	4	A1AT7	C22-C21	4.42	1.44	1.35
2	I	4	A1AT7	CB-CA	4.18	1.56	1.51
2	I	1	A1AT6	C19-N	4.14	1.46	1.39
2	I	4	A1AT7	C20-C21	2.28	1.49	1.44
2	H	4	A1AT7	C20-C21	2.23	1.49	1.44

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1	A1AT6	C23-C18-C19	-14.26	112.48	119.67
2	F	1	A1AT6	C23-C18-C19	-13.49	112.87	119.67
2	I	1	A1AT6	C23-C18-C19	-12.26	113.49	119.67
2	G	4	A1AT7	C20-C21-C22	-11.53	106.61	120.96
2	H	1	A1AT6	C23-C18-C19	-10.77	114.24	119.67
2	I	4	A1AT7	C20-C21-C22	-10.46	107.94	120.96
2	F	4	A1AT7	C20-C21-C22	-9.75	108.83	120.96
2	H	4	A1AT7	C20-C21-C22	-8.74	110.09	120.96
2	G	4	A1AT7	C27-CB-C20	-8.13	111.86	119.41
2	H	1	A1AT6	CB-CA-N	7.93	111.07	101.22
2	I	1	A1AT6	CB-CA-N	7.84	110.96	101.22
2	H	4	A1AT7	C27-CB-C20	-7.39	112.54	119.41
2	G	1	A1AT6	CB-CA-N	6.90	109.79	101.22
2	I	4	A1AT7	C26-C24-C23	6.68	127.82	117.96
2	F	1	A1AT6	CB-CA-N	6.39	109.16	101.22
2	F	4	A1AT7	C26-C24-C23	6.27	127.21	117.96
2	G	4	A1AT7	C26-C24-C23	6.24	127.17	117.96
2	F	4	A1AT7	C27-CB-C20	-5.97	113.86	119.41
2	G	1	A1AT6	C21-C22-C23	5.91	127.53	120.24
2	H	4	A1AT7	C26-C24-C23	5.74	126.43	117.96
2	I	4	A1AT7	C27-CB-C20	-5.55	114.25	119.41
2	H	1	A1AT6	C20-C19-C18	-5.47	115.51	122.12
2	F	1	A1AT6	CB-C18-C23	5.24	138.98	129.17
2	H	1	A1AT6	C22-C21-C20	5.20	126.65	120.24
2	G	1	A1AT6	CB-C18-C23	5.18	138.87	129.17
2	I	1	A1AT6	C22-C21-C20	5.07	126.50	120.24
2	F	1	A1AT6	C21-C22-C23	5.05	126.47	120.24
2	I	1	A1AT6	C21-C22-C23	4.99	126.40	120.24
2	G	4	A1AT7	C27-CB-CA	4.81	128.78	119.75
2	F	4	A1AT7	C26-C27-CB	-4.68	113.37	121.12
2	H	1	A1AT6	CB-C18-C23	4.60	137.79	129.17
2	F	1	A1AT6	C20-C19-N	4.56	134.16	127.98
2	F	1	A1AT6	C20-C19-C18	-4.53	116.64	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	A1AT6	C21-C22-C23	4.53	125.83	120.24
2	I	1	A1AT6	CB-C18-C23	4.49	137.59	129.17
2	I	1	A1AT6	C20-C19-C18	-4.37	116.84	122.12
2	H	1	A1AT6	C20-C19-N	4.32	133.84	127.98
2	I	4	A1AT7	C26-C27-CB	-4.31	113.99	121.12
2	F	4	A1AT7	C27-C26-C24	4.29	126.31	121.37
2	F	1	A1AT6	C22-C21-C20	4.26	125.50	120.24
2	G	4	A1AT7	C25-C24-C23	-4.17	115.28	120.92
2	I	1	A1AT6	C20-C19-N	4.15	133.61	127.98
2	G	1	A1AT6	C20-C19-N	4.10	133.54	127.98
2	G	4	A1AT7	C26-C27-CB	-4.02	114.47	121.12
2	G	1	A1AT6	C20-C19-C18	-4.01	117.28	122.12
2	I	4	A1AT7	C27-CB-CA	3.85	126.98	119.75
2	H	4	A1AT7	C26-C27-CB	-3.77	114.88	121.12
2	H	4	A1AT7	C27-C26-C24	3.74	125.68	121.37
2	G	4	A1AT7	C27-C26-C24	3.71	125.64	121.37
2	G	1	A1AT6	C22-C21-C20	3.69	124.79	120.24
2	F	4	A1AT7	CB-C20-C21	3.57	122.78	118.91
2	H	4	A1AT7	C27-CB-CA	3.50	126.33	119.75
2	H	4	A1AT7	CB-C20-C21	3.46	122.66	118.91
2	H	4	A1AT7	C21-C22-N	3.30	128.22	121.06
2	I	1	A1AT6	C21-C20-C19	-3.29	111.99	118.69
2	I	4	A1AT7	C27-C26-C24	3.27	125.14	121.37
2	G	4	A1AT7	C21-C22-N	3.23	128.07	121.06
2	F	1	A1AT6	C22-C23-C18	3.23	125.61	120.88
2	I	4	A1AT7	C25-C24-C23	-3.08	116.75	120.92
2	I	5	ASJ	CB-CA-C	-3.06	106.68	112.21
2	F	4	A1AT7	C21-C22-N	3.02	127.60	121.06
2	H	1	A1AT6	C21-C20-C19	-2.95	112.68	118.69
2	G	1	A1AT6	C22-C23-C18	2.92	125.15	120.88
2	G	1	A1AT6	C21-C20-C19	-2.91	112.76	118.69
2	H	1	A1AT6	C22-C23-C18	2.88	125.09	120.88
2	I	4	A1AT7	C23-C20-CB	-2.86	115.65	118.86
2	F	1	A1AT6	C21-C20-C19	-2.84	112.91	118.69
2	H	4	A1AT7	C25-C24-C23	-2.82	117.09	120.92
2	F	4	A1AT7	C27-CB-CA	2.82	125.05	119.75
2	I	4	A1AT7	CB-C20-C21	2.79	121.93	118.91
2	F	2	UN1	C6-C1-C1'	-2.72	107.42	114.51
2	I	1	A1AT6	C22-C23-C18	2.66	124.78	120.88
2	H	5	ASJ	CB-CA-C	-2.56	107.59	112.21
2	F	4	A1AT7	C25-C24-C26	-2.40	114.89	120.96
2	G	5	ASJ	OD1-CG-CB	2.35	121.30	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	2	UN1	C6-C1-C1'	-2.33	108.42	114.51
2	F	4	A1AT7	C23-C20-CB	-2.32	116.25	118.86
2	F	4	A1AT7	C25-C24-C23	-2.23	117.90	120.92
2	H	4	A1AT7	C23-C20-CB	-2.20	116.40	118.86
2	H	1	A1AT6	O-C-CA	-2.19	119.14	124.77
2	I	4	A1AT7	C25-C24-C26	-2.18	115.43	120.96
2	F	5	ASJ	OD1-CG-CB	2.18	120.78	114.00

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	2	UN1	C6-C5-CA-C
2	I	2	UN1	C6-C5-CA-N
2	F	5	ASJ	C-CA-CB-CG
2	F	5	ASJ	N-CA-CB-CG
2	G	5	ASJ	O-C-CA-N
2	G	5	ASJ	O-C-CA-CB
2	G	5	ASJ	C-CA-CB-CG
2	H	5	ASJ	C-CA-CB-CG
2	I	5	ASJ	O-C-CA-N
2	I	5	ASJ	C-CA-CB-CG
2	I	5	ASJ	N-CA-CB-CG
2	F	2	UN1	CA-C5-C6-C1
2	H	2	UN1	CA-C5-C6-C1
2	I	2	UN1	CA-C5-C6-C1
2	I	5	ASJ	O-C-CA-CB
2	G	5	ASJ	N-CA-CB-CG
2	H	5	ASJ	N-CA-CB-CG
2	H	5	ASJ	O-C-CA-N
2	H	2	UN1	C1'-C1-C6-C5
2	I	2	UN1	C6-C1-C1'-O2'
2	G	5	ASJ	CA-CB-CG-OD1
2	G	5	ASJ	CA-CB-CG-OD2
2	I	2	UN1	C6-C1-C1'-O1'
2	F	2	UN1	C6-C1-C1'-O2'
2	F	2	UN1	C6-C1-C1'-O1'

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	5	ASJ	6	0
2	F	5	ASJ	2	0
2	G	1	A1AT6	1	0
2	F	1	A1AT6	1	0
2	H	1	A1AT6	1	0

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 ⓘ

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	237/282 (84%)	0.36	14 (5%)	28 32	10, 32, 52, 68	2 (0%)
1	B	252/282 (89%)	0.17	12 (4%)	35 41	11, 29, 54, 81	2 (0%)
1	C	238/282 (84%)	0.31	11 (4%)	37 43	12, 32, 54, 71	2 (0%)
1	D	237/282 (84%)	0.15	7 (2%)	52 59	10, 29, 48, 77	3 (1%)
2	F	1/5 (20%)	2.20	1 (100%)	0 0	61, 61, 61, 61	0
2	G	1/5 (20%)	2.69	1 (100%)	0 0	55, 55, 55, 55	0
2	H	1/5 (20%)	2.81	1 (100%)	0 0	58, 58, 58, 58	0
2	I	1/5 (20%)	1.81	0	100 100	48, 48, 48, 48	0
All	All	968/1148 (84%)	0.26	47 (4%)	35 41	10, 30, 53, 81	9 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	TYR	4.7
1	B	176[A]	SER	3.9
1	D	162	GLU	3.7
1	A	97	GLY	3.4
1	A	100	PHE	3.4
1	B	98	THR	3.4
1	A	96	PRO	3.3
1	A	184	LEU	3.1
1	D	274	THR	3.1
1	A	272	ASP	3.0
1	B	162	GLU	3.0
1	C	96	PRO	2.9
1	B	161	GLY	2.9
1	C	136	HIS	2.8
1	C	273	GLU	2.8
2	H	3	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	137	PHE	2.8
2	G	3	VAL	2.7
1	D	184	LEU	2.6
1	C	98	THR	2.6
1	B	160	THR	2.5
1	D	160	THR	2.5
1	B	163	LYS	2.5
1	C	54	THR	2.4
1	B	54	THR	2.4
1	D	161	GLY	2.4
1	C	272	ASP	2.4
1	A	98	THR	2.4
1	A	99	GLU	2.3
1	A	273	GLU	2.3
1	B	47	GLY	2.3
1	B	272	ASP	2.3
2	F	3	VAL	2.2
1	A	54	THR	2.2
1	B	100	PHE	2.1
1	D	138	GLN	2.1
1	B	169	SER	2.1
1	D	163	LYS	2.1
1	C	99	GLU	2.1
1	C	100	PHE	2.1
1	C	137	PHE	2.1
1	A	95	ALA	2.1
1	C	214	ARG	2.1
1	B	55	LYS	2.0
1	C	121	PRO	2.0
1	A	139	LEU	2.0
1	A	274	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	A1AT6	H	1	11/12	0.62	0.22	67,71,80,83	0
2	A1AT6	G	1	11/12	0.76	0.17	54,58,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1AT6	F	1	11/12	0.78	0.21	56,66,74,74	0
2	A1AT7	F	4	13/14	0.80	0.16	48,56,63,65	0
2	ASJ	I	5	8/8	0.83	0.13	41,48,52,58	0
2	A1AT7	G	4	13/14	0.85	0.13	50,56,63,64	0
2	A1AT7	H	4	13/14	0.86	0.13	49,55,63,65	0
2	ASJ	H	5	8/8	0.87	0.14	51,57,64,67	0
2	A1AT6	I	1	11/12	0.87	0.12	37,43,51,52	0
2	ASJ	F	5	8/8	0.88	0.14	56,58,64,67	0
2	UN1	G	2	10/11	0.88	0.12	50,58,60,60	0
2	A1AT7	I	4	13/14	0.88	0.12	44,48,53,56	0
2	UN1	F	2	10/11	0.91	0.10	44,50,66,73	0
2	ASJ	G	5	8/8	0.91	0.11	46,50,56,59	0
2	UN1	H	2	10/11	0.92	0.12	42,55,57,65	0
2	UN1	I	2	10/11	0.93	0.08	29,37,44,49	0

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.