



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:07 AM UTC

PDB ID : 9F7M / pdb_00009f7m
Title : Blastococcus Orn bound to pGG
Authors : Mortensen, S.; Sondermann, H.
Deposited on : 2024-05-04
Resolution : 1.65 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:

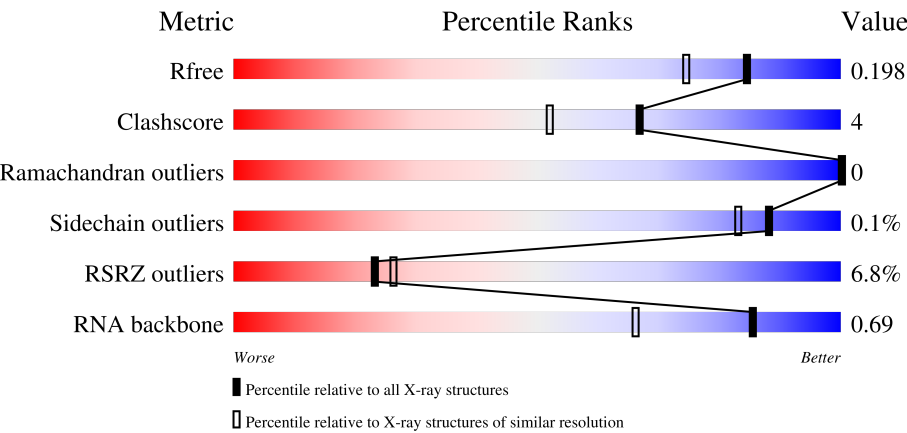
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)
RNA backbone	3983	1010 (2.16-1.16)

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	219	4% 83%11%6%
1	B	219	% 87%6%7%
1	C	219	2% 85%6%9%
1	D	219	3% 89%8%.

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Mol	Chain	Length	Quality of chain
1	E	219	
1	F	219	
1	G	219	
1	H	219	
2	I	2	
2	J	2	
2	K	2	
2	L	2	
2	M	2	
2	N	2	
2	O	2	
2	P	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15031 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 Oligoribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1586	998	277	304	7			
1	B	204	Total	C	N	O	S	0	0	0
			1582	996	276	303	7			
1	C	200	Total	C	N	O	S	0	0	0
			1548	975	267	299	7			
1	D	211	Total	C	N	O	S	0	0	0
			1627	1020	283	316	8			
1	E	209	Total	C	N	O	S	0	0	0
			1612	1013	281	310	8			
1	F	205	Total	C	N	O	S	0	0	0
			1588	999	277	305	7			
1	G	209	Total	C	N	O	S	0	0	0
			1612	1013	281	310	8			
1	H	209	Total	C	N	O	S	0	0	0
			1615	1014	281	312	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP A0A285UWY4
A	1	MET	-	expression tag	UNP A0A285UWY4
B	0	SER	-	expression tag	UNP A0A285UWY4
B	1	MET	-	expression tag	UNP A0A285UWY4
C	0	SER	-	expression tag	UNP A0A285UWY4
C	1	MET	-	expression tag	UNP A0A285UWY4
D	0	SER	-	expression tag	UNP A0A285UWY4
D	1	MET	-	expression tag	UNP A0A285UWY4
E	0	SER	-	expression tag	UNP A0A285UWY4
E	1	MET	-	expression tag	UNP A0A285UWY4
F	0	SER	-	expression tag	UNP A0A285UWY4
F	1	MET	-	expression tag	UNP A0A285UWY4
G	0	SER	-	expression tag	UNP A0A285UWY4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	expression tag	UNP A0A285UWY4
H	0	SER	-	expression tag	UNP A0A285UWY4
H	1	MET	-	expression tag	UNP A0A285UWY4

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	J	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	K	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	L	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	M	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	N	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	O	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			
2	P	2	Total	C	N	O	P	0	0	0
			47	20	10	15	2			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	I	1	Total	Na	0	0
			1	1		
3	J	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	K	1	Total	Na	0	0
			1	1		
3	L	1	Total	Na	0	0
			1	1		
3	M	1	Total	Na	0	0
			1	1		
3	N	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total 1	Na 1	0	0
3	P	1	Total 1	Na 1	0	0

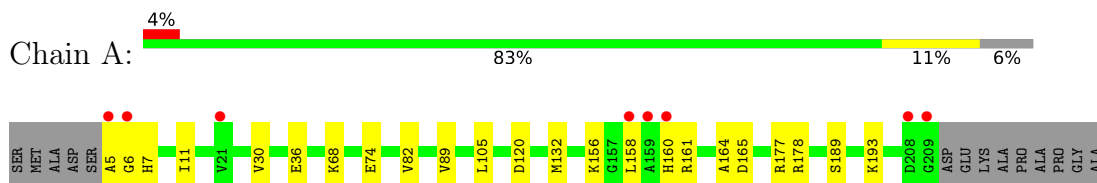
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total 244	O 244	0	0
4	I	11	Total 11	O 11	0	0
4	B	253	Total 253	O 253	0	0
4	J	15	Total 15	O 15	0	0
4	C	243	Total 243	O 243	0	0
4	K	10	Total 10	O 10	0	0
4	D	229	Total 229	O 229	0	0
4	L	12	Total 12	O 12	0	0
4	E	238	Total 238	O 238	0	0
4	M	15	Total 15	O 15	0	0
4	F	222	Total 222	O 222	0	0
4	N	10	Total 10	O 10	0	0
4	G	183	Total 183	O 183	0	0
4	O	11	Total 11	O 11	0	0
4	H	167	Total 167	O 167	0	0
4	P	12	Total 12	O 12	0	0

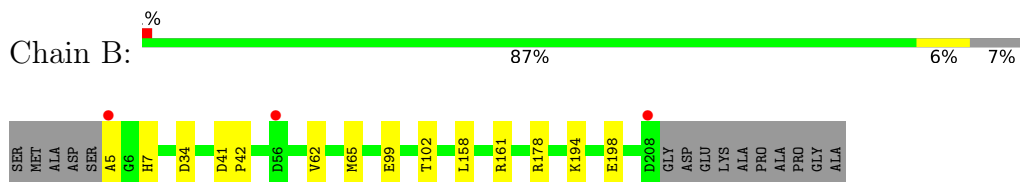
3 Residue-property plots [i](#)

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.

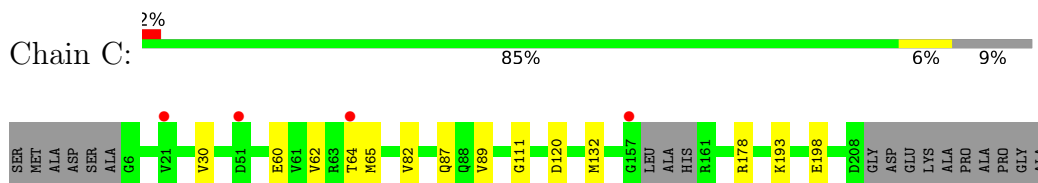
- Molecule 1: Oligoribonuclease



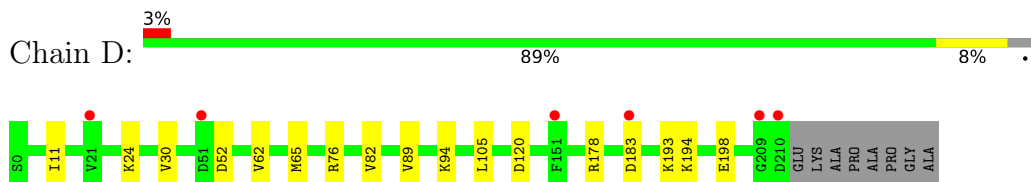
- Molecule 1: Oligoribonuclease



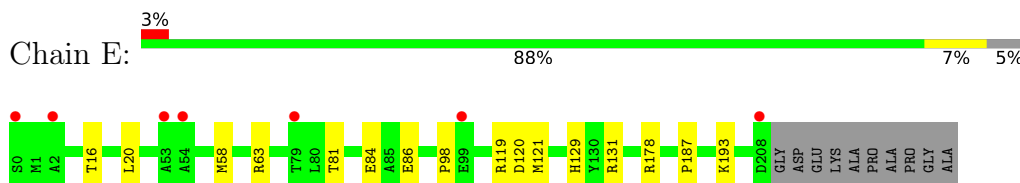
- Molecule 1: Oligoribonuclease



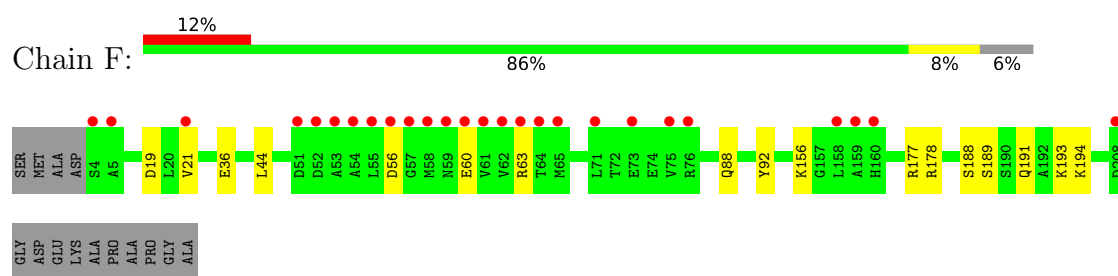
- Molecule 1: Oligoribonuclease



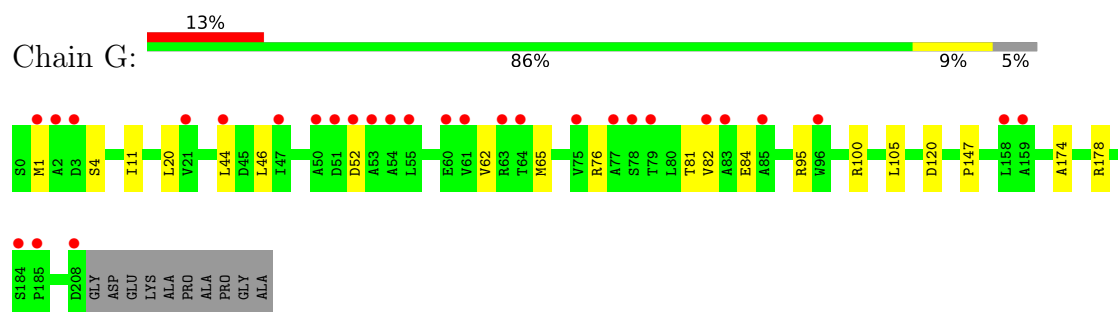
- Molecule 1: Oligoribonuclease



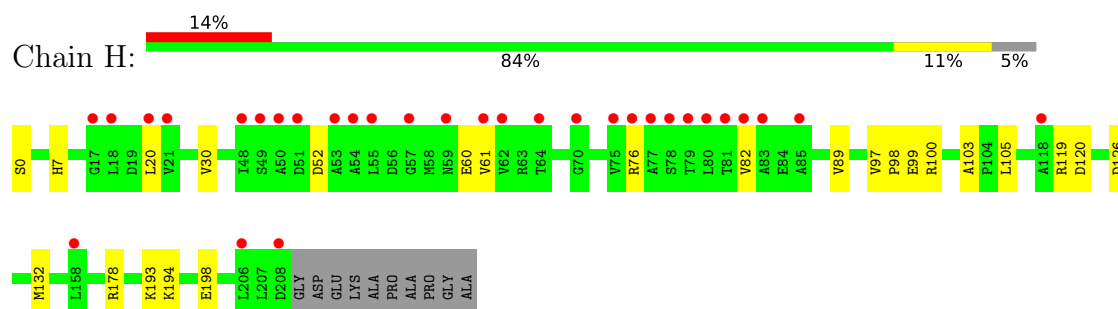
- Molecule 1: Oligoribonuclease



- Molecule 1: Oligoribonuclease



- Molecule 1: Oligoribonuclease



- Molecule 2: RNA (5'-R(P*GP*G)-3')

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*GP*G)-3')

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*GP*G)-3')

Chain K:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*GP*G)-3')

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*GP*G)-3')

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*GP*G)-3')

Chain N:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*GP*G)-3')

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: RNA (5'-R(P*GP*G)-3')

Chain P:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.57Å 117.70Å 99.47Å 90.00° 93.62° 90.00°	Depositor
Resolution (Å)	47.28 – 1.65 47.28 – 1.65	Depositor EDS
% Data completeness (in resolution range)	98.2 (47.28-1.65) 92.3 (47.28-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.171 , 0.191 0.180 , 0.198	Depositor DCC
R_{free} test set	1985 reflections (0.83%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15031	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: NA

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	0.27	0/1614	0.49	0/2190
1	B	0.29	0/1610	0.51	0/2185
1	C	0.26	0/1574	0.49	0/2135
1	D	0.28	0/1655	0.54	0/2245
1	E	0.29	0/1640	0.52	0/2225
1	F	0.28	0/1616	0.50	0/2193
1	G	0.26	0/1640	0.48	0/2225
1	H	0.24	0/1643	0.46	0/2229
2	I	0.37	0/52	0.73	0/78
2	J	0.34	0/52	0.68	0/78
2	K	0.34	0/52	0.67	0/78
2	L	0.39	0/52	0.66	0/78
2	M	0.27	0/52	0.66	0/78
2	N	0.36	0/52	0.64	0/78
2	O	0.29	0/52	0.62	0/78
2	P	0.31	0/52	0.56	0/78
All	All	0.27	0/13408	0.51	0/18251

There are no bond length outliers.

There are no bond angle outliers.

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	1586	0	1579	19	0
1	B	1582	0	1576	10	0
1	C	1548	0	1536	9	0
1	D	1627	0	1614	12	0
1	E	1612	0	1605	14	0
1	F	1588	0	1581	11	0
1	G	1612	0	1605	13	0
1	H	1615	0	1607	16	0
2	I	47	0	23	0	0
2	J	47	0	23	0	0
2	K	47	0	23	0	0
2	L	47	0	23	0	0
2	M	47	0	23	0	0
2	N	47	0	23	0	0
2	O	47	0	23	0	0
2	P	47	0	23	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	244	0	0	6	0
4	B	253	0	0	2	0
4	C	243	0	0	1	0
4	D	229	0	0	4	0
4	E	238	0	0	2	0
4	F	222	0	0	4	0
4	G	183	0	0	3	0
4	H	167	0	0	1	0
4	I	11	0	0	0	0
4	J	15	0	0	0	0
4	K	10	0	0	0	0
4	L	12	0	0	0	0
4	M	15	0	0	0	0
4	N	10	0	0	0	0
4	O	11	0	0	0	0
4	P	12	0	0	0	0
All	All	15031	0	12887	95	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 4.

All (95) 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:F:60:GLU:OE1	1:F:63:ARG:NH2	2.13	0.82
1:D:24:LYS:NZ	4:D:1401:HOH:O	2.14	0.79
1:A:74:GLU:OE2	1:A:161:ARG:NH2	2.16	0.77
1:G:1:MET:SD	4:G:301:HOH:O	2.43	0.76
1:E:20:LEU:O	1:E:119:ARG:NH1	2.19	0.75
1:G:100:ARG:NH1	4:G:301:HOH:O	2.14	0.71
1:C:87:GLN:NE2	4:C:401:HOH:O	2.25	0.69
1:F:88:GLN:OE1	4:F:301:HOH:O	2.11	0.69
1:B:178:ARG:HH11	1:B:178:ARG:HG3	1.58	0.67
1:F:178:ARG:NH1	4:F:303:HOH:O	2.28	0.66
1:C:60:GLU:O	1:C:64:THR:HG23	1.95	0.66
1:A:5:ALA:O	4:A:401:HOH:O	2.13	0.66
1:F:189:SER:O	1:F:193:LYS:HG3	1.98	0.64
1:B:7:HIS:HD2	1:B:34:ASP:HA	1.61	0.64
1:D:52:ASP:OD1	1:D:76:ARG:NH1	2.30	0.64
1:C:30:VAL:HG21	1:C:89:VAL:HG13	1.81	0.62
1:D:178:ARG:HH22	1:E:178:ARG:HH12	1.47	0.62
1:A:158:LEU:HD11	1:E:98:PRO:CB	2.30	0.61
1:A:36:GLU:OE1	1:A:177:ARG:NH1	2.24	0.61
1:E:16:THR:HB	1:E:58:MET:HG2	1.83	0.61
1:H:82:VAL:HG11	1:H:120:ASP:HB3	1.83	0.60
1:F:194:LYS:NZ	4:F:305:HOH:O	2.33	0.60
1:B:5:ALA:N	4:B:303:HOH:O	2.35	0.60
1:A:82:VAL:HG11	1:A:120:ASP:HB3	1.82	0.59
1:E:81:THR:OG1	1:E:84:GLU:HG3	2.03	0.59
1:E:119:ARG:NH2	1:E:120:ASP:OD2	2.31	0.59
1:A:68:LYS:NZ	4:A:406:HOH:O	2.32	0.58
1:D:193:LYS:NZ	4:D:1409:HOH:O	2.37	0.58
1:G:82:VAL:HG11	1:G:120:ASP:HB3	1.86	0.58
1:E:86:GLU:HB2	1:E:121:MET:HG2	1.84	0.58
1:G:95:ARG:NH1	4:G:302:HOH:O	2.25	0.58
1:A:6:GLY:O	1:A:7:HIS:ND1	2.36	0.57
1:H:20:LEU:O	1:H:119:ARG:NH1	2.32	0.57
1:D:183:ASP:OD1	4:D:1402:HOH:O	2.18	0.56
1:C:178:ARG:NH1	1:H:198:GLU:OE2	2.39	0.55
1:F:19:ASP:OD1	1:F:21:VAL:HG22	2.07	0.55
1:A:7:HIS:N	4:A:401:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:HG21	1:A:89:VAL:HG13	1.89	0.54
1:A:11:ILE:HG12	1:A:30:VAL:HG22	1.89	0.54
1:B:178:ARG:HG3	1:B:178:ARG:NH1	2.23	0.53
1:B:194:LYS:O	1:B:198:GLU:HG3	2.10	0.52
1:C:198:GLU:OE1	1:H:178:ARG:NH1	2.43	0.52
1:H:0:SER:N	1:H:99:GLU:OE2	2.30	0.52
1:F:188:SER:OG	1:F:191:GLN:HG3	2.10	0.52
1:A:158:LEU:HD11	1:E:98:PRO:HB3	1.92	0.51
1:A:5:ALA:N	4:A:408:HOH:O	2.43	0.50
1:F:156:LYS:O	1:H:98:PRO:HG2	2.10	0.50
1:A:178:ARG:HH11	1:A:178:ARG:HG3	1.77	0.50
1:C:111:GLY:HA2	1:C:132:MET:HE1	1.92	0.50
1:F:36:GLU:OE1	1:F:177:ARG:NH1	2.39	0.49
1:A:158:LEU:HD11	1:E:98:PRO:HB2	1.95	0.49
1:D:194:LYS:O	1:D:198:GLU:HG3	2.13	0.49
1:H:105:LEU:O	1:H:132:MET:HB3	2.12	0.48
1:D:94:LYS:NZ	4:D:1414:HOH:O	2.46	0.48
1:G:44:LEU:HD11	1:G:46:LEU:HD21	1.96	0.48
1:G:174:ALA:O	1:G:178:ARG:HG3	2.13	0.47
1:A:105:LEU:O	1:A:132:MET:HB3	2.15	0.47
1:F:56:ASP:OD1	4:F:302:HOH:O	2.20	0.47
1:B:198:GLU:OE2	1:E:178:ARG:NH1	2.48	0.46
1:B:62:VAL:HA	1:B:65:MET:HG2	1.97	0.46
1:G:178:ARG:HH12	1:H:178:ARG:HH12	1.62	0.46
1:H:52:ASP:OD2	1:H:76:ARG:NH1	2.47	0.46
4:B:337:HOH:O	1:E:187:PRO:HG3	2.17	0.45
1:H:193:LYS:HE3	1:H:193:LYS:HB2	1.69	0.45
1:B:99:GLU:HB3	1:B:102:THR:HG21	1.98	0.45
1:E:193:LYS:NZ	4:E:305:HOH:O	2.47	0.45
1:C:82:VAL:HG11	1:C:120:ASP:HB3	1.97	0.45
1:D:11:ILE:HB	1:D:105:LEU:HD11	1.99	0.45
1:H:60:GLU:HG2	1:H:61:VAL:N	2.31	0.44
1:G:81:THR:OG1	1:G:84:GLU:HG3	2.17	0.44
1:D:30:VAL:HG21	1:D:89:VAL:HG13	1.98	0.44
1:F:44:LEU:HD12	1:F:92:TYR:CG	2.52	0.43
1:H:97:VAL:HG11	1:H:103:ALA:HB2	2.00	0.43
1:B:161:ARG:HA	1:B:161:ARG:HD2	1.78	0.43
1:D:82:VAL:HG11	1:D:120:ASP:HB3	2.00	0.43
1:A:156:LYS:HE3	4:A:405:HOH:O	2.18	0.43
1:D:62:VAL:HA	1:D:65:MET:CG	2.49	0.43
1:B:41:ASP:CG	1:B:42:PRO:HD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:63:ARG:NH2	4:E:309:HOH:O	2.52	0.42
1:D:62:VAL:HA	1:D:65:MET:HG2	2.00	0.42
4:A:470:HOH:O	1:G:147:PRO:HD2	2.19	0.42
1:G:52:ASP:OD2	1:G:76:ARG:NH1	2.46	0.42
1:H:30:VAL:HG21	1:H:89:VAL:HG13	2.02	0.42
1:C:62:VAL:HA	1:C:65:MET:HG2	2.01	0.41
1:C:193:LYS:HB3	1:C:193:LYS:HE2	1.53	0.41
1:G:62:VAL:HA	1:G:65:MET:HG2	2.02	0.41
1:H:7:HIS:HE1	4:H:430:HOH:O	2.02	0.41
1:A:160:HIS:NE2	1:A:165:ASP:OD1	2.48	0.41
1:A:189:SER:O	1:A:193:LYS:HG3	2.20	0.41
1:E:129:HIS:CE1	1:E:131:ARG:HG3	2.56	0.41
1:G:20:LEU:HD23	1:G:20:LEU:HA	1.92	0.41
1:H:100:ARG:NH1	1:H:126:ASP:OD1	2.54	0.41
1:G:11:ILE:HB	1:G:105:LEU:HD11	2.03	0.40
1:A:160:HIS:CD2	1:A:164:ALA:HB3	2.56	0.40
1:H:194:LYS:O	1:H:198:GLU:HG3	2.22	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	203/219 (93%)	202 (100%)	1 (0%)	0	100	100
1	B	202/219 (92%)	200 (99%)	2 (1%)	0	100	100
1	C	196/219 (90%)	195 (100%)	1 (0%)	0	100	100
1	D	209/219 (95%)	206 (99%)	3 (1%)	0	100	100
1	E	207/219 (94%)	205 (99%)	2 (1%)	0	100	100
1	F	203/219 (93%)	201 (99%)	2 (1%)	0	100	100
1	G	207/219 (94%)	206 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	207/219 (94%)	206 (100%)	1 (0%)	0	100	100
All	All	1634/1752 (93%)	1621 (99%)	13 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	168/177 (95%)	168 (100%)	0	100	100
1	B	168/177 (95%)	167 (99%)	1 (1%)	78	68
1	C	165/177 (93%)	165 (100%)	0	100	100
1	D	173/177 (98%)	173 (100%)	0	100	100
1	E	171/177 (97%)	171 (100%)	0	100	100
1	F	169/177 (96%)	169 (100%)	0	100	100
1	G	171/177 (97%)	170 (99%)	1 (1%)	78	68
1	H	172/177 (97%)	172 (100%)	0	100	100
All	All	1357/1416 (96%)	1355 (100%)	2 (0%)	88	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	158	LEU
1	G	4	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	7	HIS
1	C	87	GLN
1	D	38	ASN

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Mol	Chain	Res	Type
1	E	7	HIS
1	G	7	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	I	1/2 (50%)	0	0
2	J	1/2 (50%)	0	0
2	K	1/2 (50%)	0	0
2	L	1/2 (50%)	0	0
2	M	1/2 (50%)	0	0
2	N	1/2 (50%)	0	0
2	O	1/2 (50%)	0	0
2	P	1/2 (50%)	0	0
All	All	8/16 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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.

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	205/219 (93%)	0.25	8 (3%) 43 48	21, 30, 48, 63	0
1	B	204/219 (93%)	0.09	3 (1%) 72 77	19, 30, 44, 58	0
1	C	200/219 (91%)	0.17	4 (2%) 65 70	21, 32, 44, 72	0
1	D	211/219 (96%)	0.22	6 (2%) 55 60	20, 31, 50, 71	0
1	E	209/219 (95%)	0.31	7 (3%) 49 53	20, 30, 42, 61	0
1	F	205/219 (93%)	0.76	26 (12%) 8 8	20, 32, 57, 72	0
1	G	209/219 (95%)	0.81	29 (13%) 6 7	20, 36, 54, 61	0
1	H	209/219 (95%)	0.90	31 (14%) 5 6	22, 37, 63, 77	0
2	I	2/2 (100%)	-0.76	0 100 100	21, 21, 21, 23	0
2	J	2/2 (100%)	-0.80	0 100 100	24, 24, 24, 27	0
2	K	2/2 (100%)	-0.70	0 100 100	24, 24, 24, 28	0
2	L	2/2 (100%)	-0.62	0 100 100	25, 25, 25, 28	0
2	M	2/2 (100%)	-0.73	0 100 100	24, 24, 24, 27	0
2	N	2/2 (100%)	-0.38	0 100 100	26, 26, 26, 32	0
2	O	2/2 (100%)	-0.54	0 100 100	27, 27, 27, 33	0
2	P	2/2 (100%)	-0.23	0 100 100	30, 30, 30, 35	0
All	All	1668/1768 (94%)	0.43	114 (6%) 23 26	19, 32, 53, 77	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	ALA	5.5
1	F	61	VAL	5.1
1	A	5	ALA	4.4
1	B	5	ALA	4.4
1	F	53	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	21	VAL	4.2
1	F	64	THR	4.2
1	G	77	ALA	4.0
1	F	57	GLY	3.9
1	D	210	ASP	3.9
1	A	158	LEU	3.8
1	F	4	SER	3.8
1	F	158	LEU	3.7
1	A	6	GLY	3.7
1	H	83	ALA	3.5
1	C	157	GLY	3.5
1	H	53	ALA	3.4
1	G	159	ALA	3.4
1	H	54	ALA	3.4
1	H	79	THR	3.4
1	F	62	VAL	3.4
1	G	184	SER	3.4
1	H	77	ALA	3.3
1	H	158	LEU	3.3
1	H	21	VAL	3.3
1	F	5	ALA	3.2
1	G	158	LEU	3.1
1	H	55	LEU	3.1
1	F	159	ALA	3.1
1	H	51	ASP	3.1
1	H	61	VAL	3.0
1	F	54	ALA	3.0
1	F	55	LEU	3.0
1	F	51	ASP	3.0
1	H	82	VAL	3.0
1	G	3	ASP	3.0
1	E	208	ASP	2.9
1	H	62	VAL	2.9
1	E	2	ALA	2.9
1	F	60	GLU	2.9
1	G	21	VAL	2.9
1	H	75	VAL	2.9
1	H	81	THR	2.8
1	A	160	HIS	2.8
1	G	53	ALA	2.8
1	H	49	SER	2.8
1	G	55	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	79	THR	2.8
1	G	185	PRO	2.7
1	G	51	ASP	2.7
1	D	209	GLY	2.7
1	G	54	ALA	2.7
1	G	60	GLU	2.6
1	B	56	ASP	2.6
1	D	183	ASP	2.6
1	H	80	LEU	2.6
1	H	50	ALA	2.6
1	H	18	LEU	2.6
1	F	58	MET	2.6
1	C	51	ASP	2.5
1	D	151	PHE	2.5
1	F	75	VAL	2.5
1	G	52	ASP	2.5
1	E	0	SER	2.5
1	H	57	GLY	2.4
1	B	208	ASP	2.4
1	F	208	ASP	2.4
1	F	160	HIS	2.4
1	G	78	SER	2.4
1	H	59	ASN	2.4
1	G	50	ALA	2.4
1	D	51	ASP	2.4
1	F	76	ARG	2.4
1	G	75	VAL	2.4
1	G	83	ALA	2.3
1	H	20	LEU	2.3
1	G	96	TRP	2.3
1	H	48	ILE	2.3
1	H	78	SER	2.3
1	H	206	LEU	2.3
1	F	59	ASN	2.3
1	H	76	ARG	2.3
1	A	209	GLY	2.3
1	G	64	THR	2.3
1	F	63	ARG	2.3
1	F	56	ASP	2.3
1	H	85	ALA	2.2
1	H	208	ASP	2.2
1	E	53	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	65	MET	2.2
1	G	47	ILE	2.2
1	G	82	VAL	2.2
1	E	54	ALA	2.2
1	G	208	ASP	2.2
1	H	118	ALA	2.2
1	F	73	GLU	2.1
1	G	44	LEU	2.1
1	F	52	ASP	2.1
1	A	21	VAL	2.1
1	D	21	VAL	2.1
1	G	2	ALA	2.1
1	F	71	LEU	2.1
1	A	208	ASP	2.1
1	C	64	THR	2.1
1	E	79	THR	2.1
1	H	64	THR	2.1
1	G	63	ARG	2.1
1	H	17	GLY	2.0
1	H	70	GLY	2.0
1	E	99	GLU	2.0
1	G	61	VAL	2.0
1	G	1	MET	2.0
1	G	85	ALA	2.0
1	C	21	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
3	NA	C	301	1/1	0.94	0.08	27,27,27,27	1
3	NA	A	301	1/1	0.96	0.06	25,25,25,25	1
3	NA	J	701	1/1	0.97	0.05	24,24,24,24	1
3	NA	K	701	1/1	0.97	0.05	22,22,22,22	1
3	NA	M	701	1/1	0.97	0.05	23,23,23,23	1
3	NA	I	701	1/1	0.98	0.04	21,21,21,21	1
3	NA	N	701	1/1	0.98	0.04	23,23,23,23	1
3	NA	O	701	1/1	0.98	0.05	22,22,22,22	1
3	NA	P	701	1/1	0.98	0.05	29,29,29,29	0
3	NA	L	701	1/1	0.99	0.03	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.