



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:59 PM UTC

PDB ID : 7OM6 / pdb_00007om6
Title : Thosea asigna virus RdRP domain in complex with RNA
Authors : Ferrero, D.S.; Falqui, M.; Verdaguer, N.
Deposited on : 2021-05-21
Resolution : 2.18 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

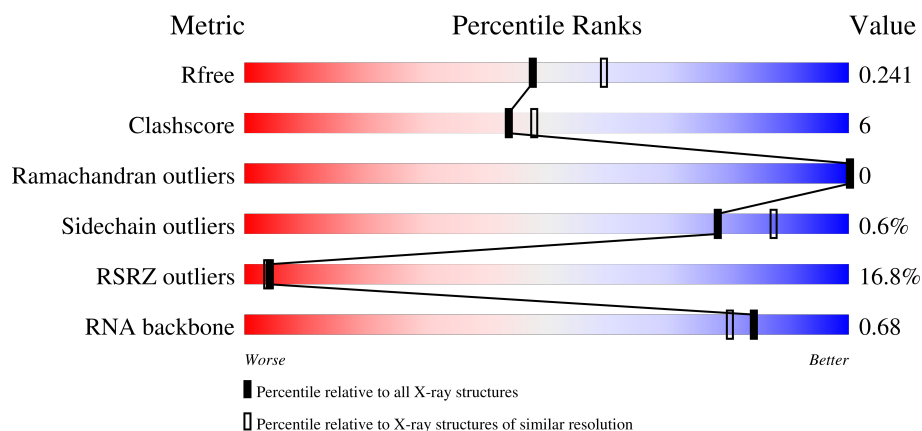
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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.



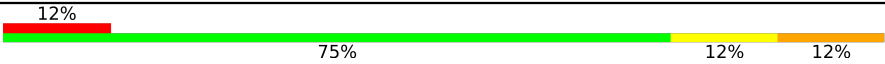
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)
RNA backbone	3983	1088 (2.50-1.86)

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	684	21% 83% 9% 8%
1	B	684	10% 84% 9% 7%
2	C	8	75% 25%
2	D	8	62% 12% 25%

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Mol	Chain	Length	Quality of chain
2	E	8	
2	F	8	

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
3	PEG	B	701	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11170 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	0	0
			4991	3164	865	936	26			
1	B	634	Total	C	N	O	S	0	0	0
			5022	3184	870	942	26			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q6A562
A	-11	GLY	-	expression tag	UNP Q6A562
A	-10	SER	-	expression tag	UNP Q6A562
A	-9	SER	-	expression tag	UNP Q6A562
A	-8	HIS	-	expression tag	UNP Q6A562
A	-7	HIS	-	expression tag	UNP Q6A562
A	-6	HIS	-	expression tag	UNP Q6A562
A	-5	HIS	-	expression tag	UNP Q6A562
A	-4	HIS	-	expression tag	UNP Q6A562
A	-3	HIS	-	expression tag	UNP Q6A562
A	-2	SER	-	expression tag	UNP Q6A562
A	-1	GLN	-	expression tag	UNP Q6A562
A	0	ASP	-	expression tag	UNP Q6A562
A	1	LEU	-	expression tag	UNP Q6A562
A	2	GLU	-	expression tag	UNP Q6A562
A	3	ASN	-	expression tag	UNP Q6A562
A	4	LEU	-	expression tag	UNP Q6A562
A	5	TYR	-	expression tag	UNP Q6A562
A	6	PHE	-	expression tag	UNP Q6A562
A	7	GLN	-	expression tag	UNP Q6A562
A	8	GLY	-	expression tag	UNP Q6A562
A	9	GLY	-	expression tag	UNP Q6A562
A	10	SER	-	expression tag	UNP Q6A562
B	-12	MET	-	initiating methionine	UNP Q6A562
B	-11	GLY	-	expression tag	UNP Q6A562

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	SER	-	expression tag	UNP Q6A562
B	-9	SER	-	expression tag	UNP Q6A562
B	-8	HIS	-	expression tag	UNP Q6A562
B	-7	HIS	-	expression tag	UNP Q6A562
B	-6	HIS	-	expression tag	UNP Q6A562
B	-5	HIS	-	expression tag	UNP Q6A562
B	-4	HIS	-	expression tag	UNP Q6A562
B	-3	HIS	-	expression tag	UNP Q6A562
B	-2	SER	-	expression tag	UNP Q6A562
B	-1	GLN	-	expression tag	UNP Q6A562
B	0	ASP	-	expression tag	UNP Q6A562
B	1	LEU	-	expression tag	UNP Q6A562
B	2	GLU	-	expression tag	UNP Q6A562
B	3	ASN	-	expression tag	UNP Q6A562
B	4	LEU	-	expression tag	UNP Q6A562
B	5	TYR	-	expression tag	UNP Q6A562
B	6	PHE	-	expression tag	UNP Q6A562
B	7	GLN	-	expression tag	UNP Q6A562
B	8	GLY	-	expression tag	UNP Q6A562
B	9	GLY	-	expression tag	UNP Q6A562
B	10	SER	-	expression tag	UNP Q6A562

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			126	57	21	42	6			
2	D	6	Total	C	N	O	P	0	0	0
			126	57	21	42	6			
2	E	8	Total	C	N	O	P	0	0	0
			168	76	29	55	8			
2	F	8	Total	C	N	O	P	0	0	0
			168	76	29	55	8			

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

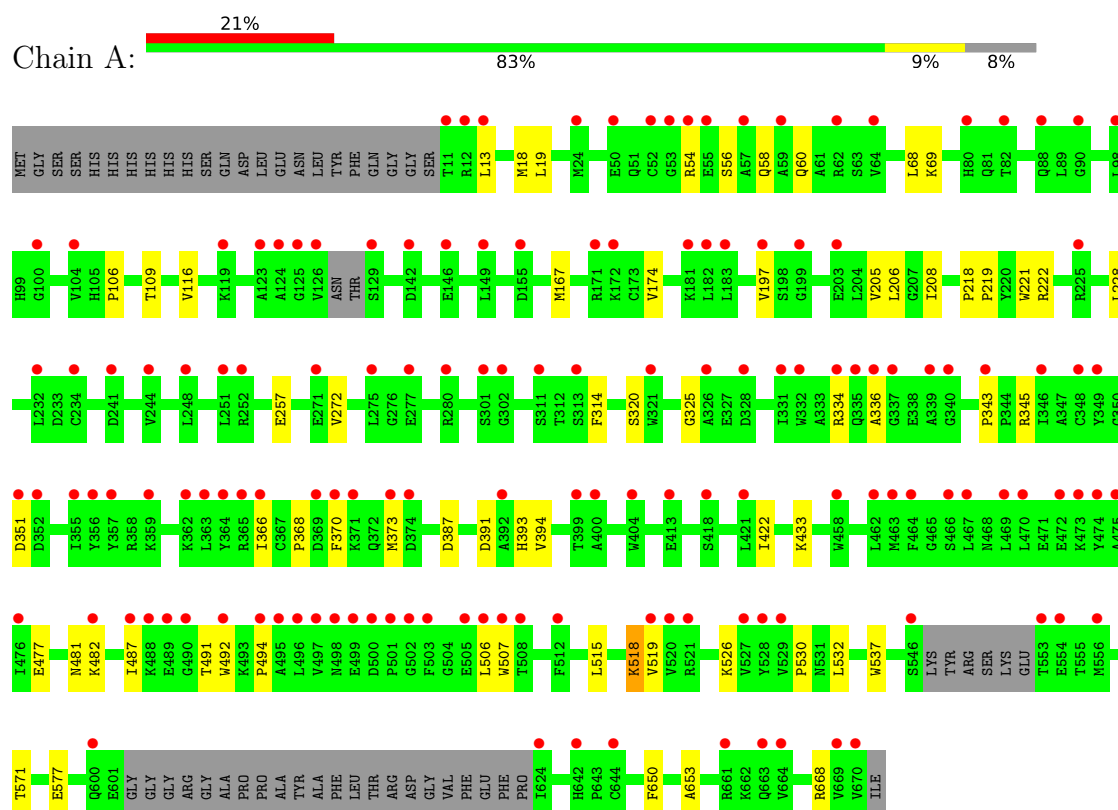
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	191	Total	O	0	0
			191	191		
4	B	309	Total	O	0	0
			309	309		
4	C	12	Total	O	0	0
			12	12		
4	D	10	Total	O	0	0
			10	10		
4	E	22	Total	O	0	0
			22	22		
4	F	11	Total	O	0	0
			11	11		

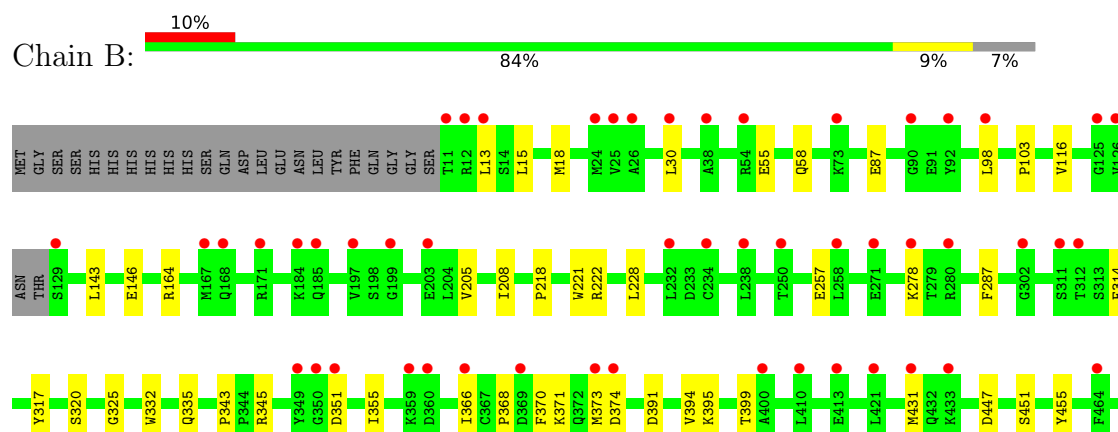
3 Residue-property plots [i](#)

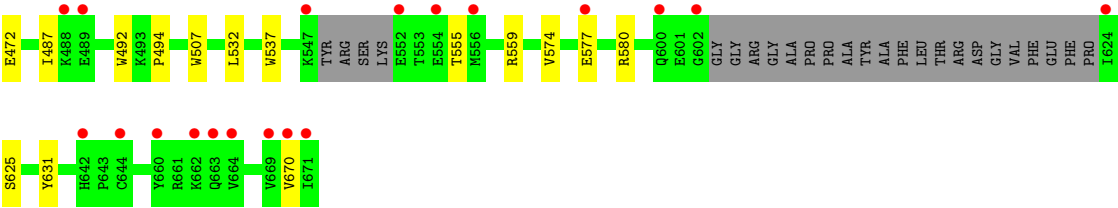
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RNA-dependent RNA polymerase



- Molecule 1: RNA-dependent RNA polymerase

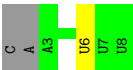




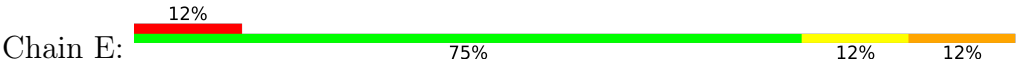
● Molecule 2: RNA (5'-R(P*AP*AP*AP*UP*UP*U)-3')



● Molecule 2: RNA (5'-R(P*AP*AP*AP*UP*UP*U)-3')



● Molecule 2: RNA (5'-R(P*AP*AP*AP*UP*UP*U)-3')



● Molecule 2: RNA (5'-R(P*AP*AP*AP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.64Å 204.03Å 70.08Å 90.00° 97.19° 90.00°	Depositor
Resolution (Å)	49.30 – 2.18 49.30 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.30-2.18) 99.1 (49.30-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.229 , 0.241 0.229 , 0.241	Depositor DCC
R_{free} test set	4544 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11170	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: PEG

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	0.89	0/5099	1.26	4/6902 (0.1%)
1	B	0.91	0/5130	1.25	5/6943 (0.1%)
2	C	0.13	0/140	0.27	0/215
2	D	0.43	0/140	0.58	0/215
2	E	0.46	0/187	0.72	1/288 (0.3%)
2	F	0.27	0/187	0.41	0/288
All	All	0.88	0/10883	1.22	10/14851 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	PRO	N-CA-C	6.48	118.61	110.70
1	A	343	PRO	N-CA-C	5.79	117.77	110.70
1	B	507	TRP	N-CA-C	-5.73	104.72	110.97
1	A	422	ILE	N-CA-C	-5.52	106.29	111.48
2	E	1	C	N1-C1'-C2'	5.42	122.14	114.00
1	B	314	PHE	N-CA-C	-5.41	106.56	112.72
1	B	317	TYR	CB-CA-C	5.37	118.83	110.67
1	B	287	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	314	PHE	N-CA-C	-5.09	106.38	112.59
1	A	507	TRP	N-CA-C	-5.02	105.70	111.07

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	4991	0	4948	76	0
1	B	5022	0	4982	62	0
2	C	126	0	64	0	0
2	D	126	0	64	1	0
2	E	168	0	86	1	0
2	F	168	0	86	2	0
3	A	7	0	10	0	0
3	B	7	0	10	5	0
4	A	191	0	0	1	1
4	B	309	0	0	2	1
4	C	12	0	0	0	0
4	D	10	0	0	0	0
4	E	22	0	0	0	0
4	F	11	0	0	2	0
All	All	11170	0	10250	127	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 6.

All (127) 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:351:ASP:HA	1:A:373:MET:HE1	1.20	1.13
1:A:370:PHE:HD2	1:A:373:MET:HE2	1.16	1.09
1:B:278:LYS:NZ	3:B:701:PEG:H21	1.66	1.07
1:B:577:GLU:OE1	1:B:580:ARG:NH2	1.91	1.04
1:A:370:PHE:CD2	1:A:373:MET:HE2	1.96	1.00
1:B:370:PHE:CE1	1:B:487:ILE:HD13	1.99	0.96
1:A:370:PHE:HD2	1:A:373:MET:CE	1.80	0.94
1:A:351:ASP:HA	1:A:373:MET:CE	1.99	0.93
1:B:370:PHE:CE1	1:B:487:ILE:CD1	2.57	0.87
1:B:278:LYS:HZ1	3:B:701:PEG:H21	1.37	0.86
1:B:278:LYS:HZ2	3:B:701:PEG:H21	1.38	0.86
1:A:370:PHE:CE1	1:A:487:ILE:HD13	2.13	0.82
1:A:370:PHE:HB2	1:A:373:MET:HE3	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:GLU:HB2	1:B:431:MET:SD	2.20	0.81
1:B:373:MET:HE1	1:B:451:SER:HB2	1.63	0.81
2:F:6:U:O2'	4:F:101:HOH:O	2.00	0.80
1:A:668:ARG:CG	1:B:399:THR:HG22	2.11	0.80
1:A:370:PHE:CE1	1:A:487:ILE:CD1	2.63	0.80
1:B:366:ILE:HG22	1:B:368:PRO:HG3	1.65	0.79
1:A:668:ARG:HG2	1:B:399:THR:HG22	1.65	0.76
1:A:370:PHE:CD1	1:A:487:ILE:HD13	2.23	0.74
1:A:370:PHE:HE1	1:A:487:ILE:CD1	2.00	0.73
1:A:668:ARG:HD3	1:B:399:THR:HG21	1.69	0.73
1:A:366:ILE:HG22	1:A:368:PRO:HG3	1.71	0.73
1:B:373:MET:HE2	1:B:447:ASP:O	1.88	0.72
1:B:370:PHE:CD1	1:B:487:ILE:HD13	2.25	0.71
1:A:370:PHE:HE1	1:A:487:ILE:HD11	1.56	0.71
1:A:351:ASP:CA	1:A:373:MET:HE1	2.11	0.70
1:B:577:GLU:OE2	4:B:801:HOH:O	2.08	0.70
1:A:366:ILE:CG2	1:A:368:PRO:HG3	2.22	0.68
1:B:366:ILE:CG2	1:B:368:PRO:HG3	2.23	0.68
1:B:370:PHE:HE1	1:B:487:ILE:CD1	2.05	0.66
2:F:7:U:OP1	4:F:102:HOH:O	2.13	0.66
1:B:366:ILE:HD11	1:B:494:PRO:HG3	1.78	0.64
1:A:370:PHE:CD2	1:A:373:MET:CE	2.68	0.64
1:A:668:ARG:HB3	1:B:399:THR:HG22	1.80	0.63
1:B:373:MET:CE	1:B:447:ASP:O	2.46	0.63
1:A:668:ARG:CB	1:B:399:THR:HG22	2.30	0.61
1:A:370:PHE:HB2	1:A:373:MET:CE	2.28	0.61
1:B:373:MET:CE	1:B:451:SER:HB2	2.31	0.60
1:B:370:PHE:CE1	1:B:487:ILE:HD11	2.36	0.60
1:A:668:ARG:CD	1:B:399:THR:HG21	2.31	0.60
1:A:366:ILE:HD11	1:A:494:PRO:HG3	1.85	0.59
1:A:477:GLU:HG3	1:A:481:ASN:ND2	2.17	0.58
1:A:519:VAL:CG1	1:A:526:LYS:HB3	2.34	0.58
1:A:477:GLU:CG	1:A:481:ASN:ND2	2.67	0.57
1:B:278:LYS:HZ2	3:B:701:PEG:C2	2.15	0.57
1:A:106:PRO:HB2	1:A:109:THR:CG2	2.35	0.56
1:A:477:GLU:HG3	1:A:481:ASN:HD21	1.71	0.55
1:B:13:LEU:HD23	1:B:18:MET:HG3	1.89	0.55
1:A:351:ASP:CA	1:A:373:MET:CE	2.79	0.54
1:B:366:ILE:CD1	1:B:494:PRO:HG3	2.38	0.54
1:A:366:ILE:HG22	1:A:368:PRO:CG	2.37	0.54
1:B:366:ILE:HG22	1:B:368:PRO:CG	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:PRO:HA	1:A:491:THR:HB	1.89	0.54
1:B:351:ASP:HA	1:B:373:MET:SD	2.48	0.54
1:A:370:PHE:CE1	1:A:487:ILE:HD11	2.37	0.54
1:A:668:ARG:HD3	1:B:399:THR:CG2	2.37	0.53
1:A:106:PRO:HB2	1:A:109:THR:HG22	1.90	0.53
1:A:228:LEU:HD22	1:B:18:MET:HE2	1.91	0.52
1:A:477:GLU:HG2	1:A:481:ASN:HD22	1.73	0.52
1:A:54:ARG:HG2	1:A:58:GLN:HE21	1.74	0.52
1:A:668:ARG:CD	1:B:399:THR:CG2	2.88	0.52
1:B:472:GLU:HG3	1:B:492:TRP:HB3	1.91	0.52
1:A:477:GLU:HG2	4:A:876:HOH:O	2.09	0.51
1:A:116:VAL:HG21	1:A:257:GLU:HG3	1.92	0.51
1:A:205:VAL:O	1:A:208:ILE:HG13	2.11	0.51
1:A:519:VAL:HG13	1:A:526:LYS:HB3	1.93	0.51
1:B:143:LEU:HA	1:B:146:GLU:OE2	2.10	0.50
1:B:205:VAL:O	1:B:208:ILE:HG13	2.11	0.50
1:B:370:PHE:HE1	1:B:487:ILE:HD11	1.71	0.50
1:B:332:TRP:O	1:B:335:GLN:HG2	2.11	0.50
1:A:668:ARG:CG	1:B:399:THR:CG2	2.86	0.49
1:B:391:ASP:HA	1:B:394:VAL:HG22	1.93	0.49
1:B:98:LEU:HD23	1:B:103:PRO:HA	1.95	0.49
1:B:87:GLU:CB	1:B:431:MET:SD	2.97	0.49
1:A:532:LEU:HB2	1:A:537:TRP:CE2	2.48	0.49
1:A:106:PRO:O	1:A:109:THR:HG22	2.14	0.48
1:B:355:ILE:HD11	1:B:455:TYR:CE1	2.48	0.48
1:B:55:GLU:HA	1:B:58:GLN:HE21	1.79	0.47
1:B:371:LYS:HG3	3:B:701:PEG:H12	1.97	0.47
1:A:218:PRO:HG3	1:A:221:TRP:CZ2	2.49	0.47
1:A:320:SER:O	1:A:325:GLY:HA3	2.15	0.47
1:A:351:ASP:CB	1:A:373:MET:CE	2.93	0.46
1:A:18:MET:HE2	1:B:228:LEU:HD22	1.97	0.46
1:A:391:ASP:HA	1:A:394:VAL:HG22	1.97	0.46
1:A:650:PHE:HB2	1:A:653:ALA:HB2	1.97	0.45
1:A:571:THR:HG21	2:D:6:U:H4'	1.99	0.45
1:A:334:ARG:C	1:A:336:ALA:H	2.25	0.45
1:A:197:VAL:HG21	1:A:393:HIS:HB3	1.99	0.44
1:A:515:LEU:HD22	1:A:530:PRO:HB2	1.99	0.44
1:A:218:PRO:HA	1:A:219:PRO:HA	1.80	0.43
1:B:116:VAL:HG21	1:B:257:GLU:HG3	2.00	0.43
1:B:366:ILE:CG1	1:B:494:PRO:HG3	2.47	0.43
1:A:68:LEU:HD11	1:A:272:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:ARG:HD3	1:B:345:ARG:HA	1.83	0.43
1:B:395:LYS:HD3	1:B:395:LYS:HA	1.83	0.43
1:B:532:LEU:HB2	1:B:537:TRP:CE2	2.53	0.43
1:A:506:LEU:HD23	1:A:518:LYS:HB2	2.00	0.43
1:A:69:LYS:HE3	1:A:69:LYS:HB3	1.88	0.43
1:B:218:PRO:HG3	1:B:221:TRP:CZ2	2.53	0.43
1:B:320:SER:O	1:B:325:GLY:HA3	2.19	0.43
2:E:1:C:H2'	2:E:1:C:O2	2.19	0.43
1:A:366:ILE:HD13	1:A:492:TRP:CE2	2.54	0.42
1:B:30:LEU:HD21	1:B:555:THR:HG21	2.01	0.42
1:A:366:ILE:CD1	1:A:494:PRO:HG3	2.48	0.42
1:A:13:LEU:HD23	1:A:18:MET:HG3	2.00	0.42
1:A:668:ARG:HG2	1:B:399:THR:CG2	2.43	0.42
1:A:167:MET:HE3	1:A:167:MET:HB2	1.90	0.42
1:A:366:ILE:HG22	1:A:368:PRO:CD	2.49	0.42
1:B:374:ASP:HB3	4:B:876:HOH:O	2.20	0.42
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.90	0.42
1:B:366:ILE:HD13	1:B:492:TRP:CE2	2.54	0.42
1:B:559:ARG:HH22	1:B:625:SER:HB3	1.85	0.42
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.92	0.41
1:A:206:LEU:HA	1:B:15:LEU:HB2	2.01	0.41
1:A:106:PRO:HB2	1:A:109:THR:HG21	2.02	0.41
1:A:668:ARG:HB3	1:B:399:THR:CG2	2.47	0.41
1:B:574:VAL:HG21	1:B:631:TYR:HA	2.01	0.41
1:A:477:GLU:HG2	1:A:481:ASN:ND2	2.32	0.41
1:A:174:VAL:HG11	1:A:482:LYS:O	2.21	0.41
1:B:164:ARG:NH2	1:B:278:LYS:HE3	2.36	0.41
1:A:56:SER:O	1:A:60:GLN:HG3	2.21	0.40
1:A:345:ARG:HD3	1:A:345:ARG:HA	1.94	0.40
1:A:351:ASP:CB	1:A:373:MET:HE3	2.51	0.40
1:A:366:ILE:HG22	1:A:368:PRO:HD3	2.02	0.40
1:B:143:LEU:O	1:B:146:GLU:HG2	2.22	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)
4:A:984:HOH:O	4:B:1072:HOH:O[1_556]	2.13	0.07

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	622/684 (91%)	612 (98%)	10 (2%)	0	100	100
1	B	626/684 (92%)	616 (98%)	10 (2%)	0	100	100
All	All	1248/1368 (91%)	1228 (98%)	20 (2%)	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	537/581 (92%)	532 (99%)	5 (1%)	70	81
1	B	540/581 (93%)	538 (100%)	2 (0%)	84	91
All	All	1077/1162 (93%)	1070 (99%)	7 (1%)	78	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	ARG
1	A	387	ASP
1	A	433	LYS
1	A	518	LYS
1	A	577	GLU
1	B	222	ARG
1	B	670	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	110	HIS
1	A	121	GLN
1	A	285	HIS
1	A	481	ASN
1	A	524	ASN
1	A	600	GLN
1	A	663	GLN
1	B	58	GLN
1	B	242	HIS
1	B	285	HIS
1	B	335	GLN
1	B	396	GLN
1	B	432	GLN
1	B	456	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	5/8 (62%)	0	0
2	D	5/8 (62%)	0	0
2	E	7/8 (87%)	1 (14%)	0
2	F	7/8 (87%)	1 (14%)	0
All	All	24/32 (75%)	2 (8%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	4	A
2	F	4	A

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
3	PEG	A	701	-	6,6,6	0.08	0	5,5,5	0.15	0
3	PEG	B	701	-	6,6,6	0.11	0	5,5,5	0.10	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	PEG	A	701	-	-	3/4/4/4	-
3	PEG	B	701	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	701	PEG	O1-C1-C2-O2
3	B	701	PEG	O1-C1-C2-O2
3	B	701	PEG	O2-C3-C4-O4
3	A	701	PEG	O2-C3-C4-O4
3	B	701	PEG	C4-C3-O2-C2
3	A	701	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	PEG	5	0

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	630/684 (92%)	1.35	145 (23%) 2 2	29, 52, 81, 112	0
1	B	634/684 (92%)	0.87	70 (11%) 10 9	24, 44, 70, 94	0
2	C	6/8 (75%)	-0.62	0 100 100	32, 34, 42, 66	0
2	D	6/8 (75%)	-0.28	0 100 100	42, 46, 56, 87	0
2	E	8/8 (100%)	-0.27	1 (12%) 8 7	37, 41, 60, 94	0
2	F	8/8 (100%)	-0.10	1 (12%) 8 7	43, 51, 69, 116	0
All	All	1292/1400 (92%)	1.08	217 (16%) 4 4	24, 48, 77, 116	0

All (217) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	VAL	6.9
1	B	126	VAL	6.7
1	A	670	VAL	5.3
1	B	11	THR	5.3
1	A	501	PRO	5.2
1	A	462	LEU	5.1
1	A	11	THR	5.1
1	B	431	MET	5.0
1	A	496	LEU	4.8
1	B	624	ILE	4.6
1	A	553	THR	4.5
1	B	602	GLY	4.4
1	A	506	LEU	4.3
1	A	363	LEU	4.3
1	A	356	TYR	4.3
1	A	373	MET	4.2
1	B	577	GLU	4.2
1	A	469	LEU	4.1
1	A	52	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	234	CYS	3.9
1	A	464	PHE	3.9
1	A	498	ASN	3.8
1	A	624	ILE	3.8
1	A	497	VAL	3.8
1	B	547	LYS	3.8
1	A	340	GLY	3.8
1	B	664	VAL	3.7
1	A	13	LEU	3.7
1	B	552	GLU	3.7
1	B	671	ILE	3.7
1	A	467	LEU	3.6
1	A	474	TYR	3.6
1	A	366	ILE	3.6
1	B	644	CYS	3.6
1	B	464	PHE	3.5
1	A	129	SER	3.5
1	B	373	MET	3.5
1	A	369	ASP	3.5
1	B	125	GLY	3.4
1	A	241	ASP	3.4
1	A	669	VAL	3.4
1	A	24	MET	3.4
1	A	520	VAL	3.3
1	B	670	VAL	3.3
1	A	644	CYS	3.3
1	A	302	GLY	3.3
1	A	473	LYS	3.3
1	A	104	VAL	3.2
1	A	88	GLN	3.2
1	A	181	LYS	3.2
1	B	400	ALA	3.2
1	A	466	SER	3.2
1	B	369	ASP	3.1
1	A	488	LYS	3.1
1	A	124	ALA	3.1
1	A	507	TRP	3.1
1	A	490	GLY	3.1
1	A	482	LYS	3.1
1	A	463	MET	3.1
1	B	663	GLN	3.1
1	B	38	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	399	THR	3.0
1	A	197	VAL	3.0
1	A	508	THR	3.0
1	B	556	MET	3.0
1	A	475	ALA	2.9
2	E	1	C	2.9
1	A	502	GLY	2.9
1	A	528	TYR	2.9
1	A	546	SER	2.9
1	B	359	LYS	2.9
1	A	252	ARG	2.9
1	B	238	LEU	2.9
1	A	277	GLU	2.8
1	B	129	SER	2.8
1	B	199	GLY	2.8
1	B	234	CYS	2.8
1	B	351	ASP	2.8
1	A	527	VAL	2.7
1	B	98	LEU	2.7
1	B	488	LYS	2.7
1	A	100	GLY	2.7
1	A	203	GLU	2.6
1	A	495	ALA	2.6
1	A	98	LEU	2.6
1	A	364	TYR	2.6
1	A	499	GLU	2.6
1	A	172	LYS	2.6
1	A	642	HIS	2.6
1	B	662	LYS	2.6
1	A	357	TYR	2.6
1	A	82	THR	2.6
1	A	326	ALA	2.6
1	A	343	PRO	2.5
1	A	400	ALA	2.5
1	A	470	LEU	2.5
1	B	25	VAL	2.5
1	A	119	LYS	2.5
1	A	500	ASP	2.5
1	A	600	GLN	2.5
1	A	505	GLU	2.5
1	A	404	TRP	2.5
1	A	487	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	529	VAL	2.5
1	B	660	TYR	2.5
1	B	271	GLU	2.5
1	A	59	ALA	2.5
1	B	421	LEU	2.5
1	A	125	GLY	2.5
1	A	271	GLU	2.4
1	A	335	GLN	2.4
1	A	556	MET	2.4
1	A	359	LYS	2.4
1	B	413	GLU	2.4
1	B	374	ASP	2.4
1	A	251	LEU	2.4
1	A	337	GLY	2.4
1	A	50	GLU	2.4
1	A	663	GLN	2.4
1	A	142	ASP	2.4
1	A	244	VAL	2.4
1	A	321	TRP	2.4
1	A	12	ARG	2.4
1	A	62	ARG	2.4
1	A	371	LYS	2.4
1	A	472	GLU	2.4
1	B	90	GLY	2.4
1	B	302	GLY	2.4
1	B	360	ASP	2.4
1	A	301	SER	2.4
1	A	332	TRP	2.4
1	A	199	GLY	2.3
1	A	370	PHE	2.3
1	B	280	ARG	2.3
1	B	554	GLU	2.3
1	B	168	GLN	2.3
1	A	275	LEU	2.3
1	A	374	ASP	2.3
1	B	278	LYS	2.3
1	A	418	SER	2.3
1	A	476	ILE	2.3
1	A	413	GLU	2.3
1	A	489	GLU	2.3
1	A	392	ALA	2.3
1	A	53	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	12	ARG	2.3
2	F	1	C	2.3
1	A	311	SER	2.3
1	B	203	GLU	2.3
1	A	331	ILE	2.3
1	A	64	VAL	2.3
1	A	123	ALA	2.3
1	B	30	LEU	2.3
1	B	92	TYR	2.3
1	A	554	GLU	2.2
1	B	366	ILE	2.2
1	A	280	ARG	2.2
1	A	155	ASP	2.2
1	A	339	ALA	2.2
1	A	248	LEU	2.2
1	B	258	LEU	2.2
1	A	313	SER	2.2
1	A	334	ARG	2.2
1	A	519	VAL	2.2
1	B	433	LYS	2.2
1	B	167	MET	2.2
1	A	90	GLY	2.2
1	A	55	GLU	2.2
1	B	26	ALA	2.2
1	A	183	LEU	2.2
1	B	232	LEU	2.2
1	B	600	GLN	2.2
1	A	661	ARG	2.2
1	B	73	LYS	2.2
1	A	346	ILE	2.2
1	A	512	PHE	2.2
1	A	146	GLU	2.2
1	B	489	GLU	2.2
1	A	149	LEU	2.2
1	A	348	CYS	2.2
1	B	54	ARG	2.2
1	B	184	LYS	2.2
1	B	197	VAL	2.1
1	B	669	VAL	2.1
1	A	182	LEU	2.1
1	A	421	LEU	2.1
1	B	13	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	24	MET	2.1
1	A	352	ASP	2.1
1	A	355	ILE	2.1
1	A	80	HIS	2.1
1	B	171	ARG	2.1
1	A	362	LYS	2.1
1	B	311	SER	2.1
1	B	410	LEU	2.1
1	B	250	THR	2.1
1	B	642	HIS	2.1
1	A	54	ARG	2.1
1	A	458	TRP	2.1
1	A	492	TRP	2.1
1	A	57	ALA	2.1
1	A	351	ASP	2.1
1	A	171	ARG	2.1
1	A	365	ARG	2.1
1	A	328	ASP	2.0
1	B	185	GLN	2.0
1	A	225	ARG	2.0
1	A	494	PRO	2.0
1	B	349	TYR	2.0
1	B	350	GLY	2.0
1	A	503	PHE	2.0
1	A	664	VAL	2.0
1	A	336	ALA	2.0
1	A	232	LEU	2.0
1	A	521	ARG	2.0
1	B	312	THR	2.0
1	A	349	TYR	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 [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
3	PEG	A	701	7/7	0.76	0.25	69,72,76,76	0
3	PEG	B	701	7/7	0.87	0.18	62,65,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.