



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:52 AM EDT

PDB ID : 1SH3 / pdb_00001sh3
Title : Crystal Structure of Norwalk Virus Polymerase (MgSO4 crystal form)
Authors : Ng, K.K.; Pendas-Franco, N.; Rojo, J.; Boga, J.A.; Machin, A.; Alonso, J.M.; Parra, F.
Deposited on : 2004-02-24
Resolution : 2.95 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

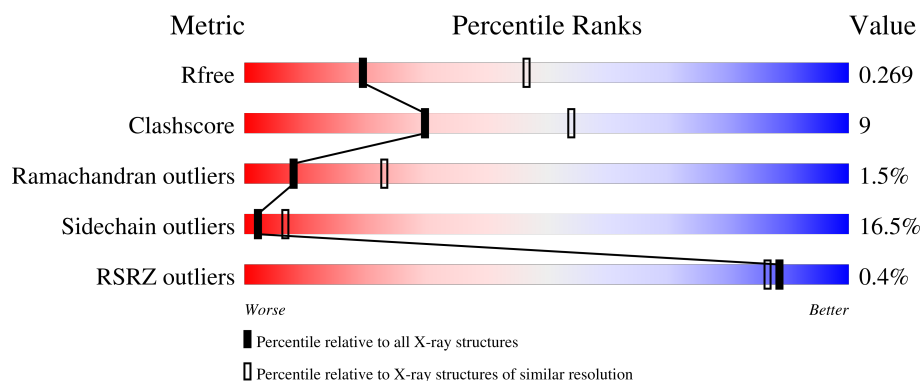
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	510	
1	B	510	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7892 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 Polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			3939	2501	675	741	22			
1	B	503	Total	C	N	O	S	0	0	0
			3948	2507	677	742	22			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

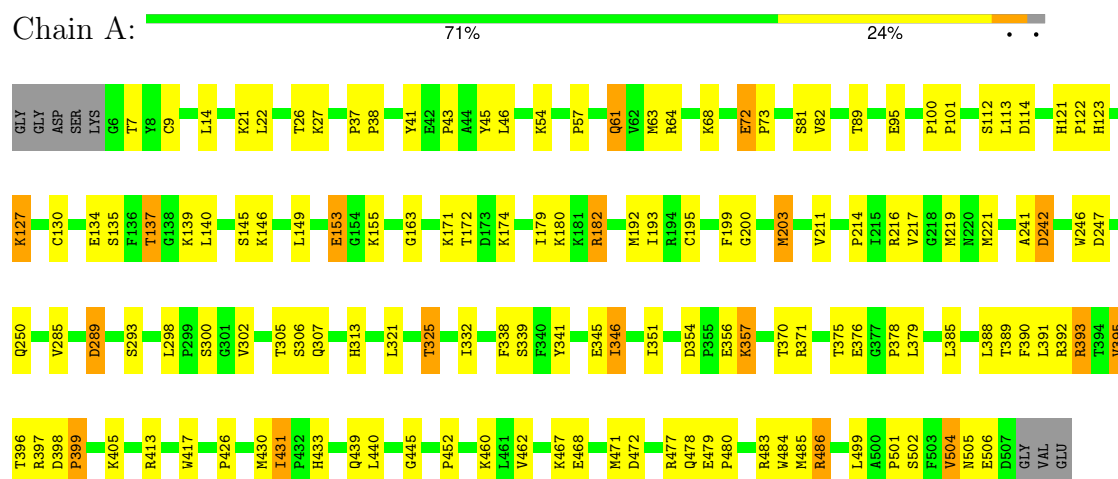
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	2	Total	O	0	0
			2	2		

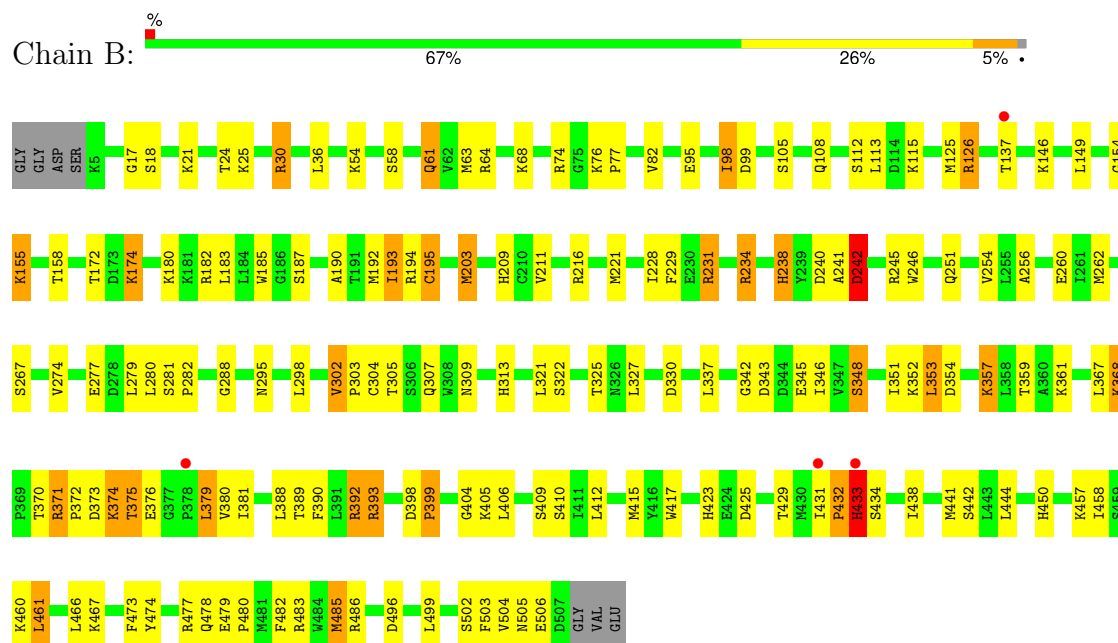
3 Residue-property plots

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: RNA Polymerase



• Molecule 1: RNA Polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.05Å 109.14Å 112.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 20.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.95) 99.6 (20.00-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.215 , 0.280 0.209 , 0.269	Depositor DCC
R_{free} test set	1419 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7892	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.55	0/4041	0.94	0/5483
1	B	0.53	0/4050	0.93	1/5494 (0.0%)
All	All	0.54	0/8091	0.93	1/10977 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	ASN	N-CA-C	5.05	117.33	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3939	0	3906	70	0
1	B	3948	0	3919	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
All	All	7892	0	7825	134	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 9.

All (134) 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:393:ARG:HG2	1:A:393:ARG:HH11	1.38	0.88
1:B:241:ALA:HA	1:B:379:LEU:HD21	1.57	0.87
1:B:398:ASP:HB2	1:B:399:PRO:HD2	1.60	0.84
1:A:9:CYS:SG	1:A:68:LYS:NZ	2.54	0.80
1:B:371:ARG:HG3	1:B:372:PRO:HD2	1.67	0.77
1:A:371:ARG:HD3	1:A:378:PRO:O	1.85	0.76
1:A:289:ASP:N	1:A:289:ASP:OD1	2.20	0.75
1:A:477:ARG:O	1:A:480:PRO:HD2	1.87	0.74
1:B:113:LEU:HD11	1:B:193:ILE:HG22	1.71	0.71
1:A:486:ARG:HG2	1:A:486:ARG:HH11	1.55	0.71
1:A:203:MET:HG3	1:A:307:GLN:OE1	1.92	0.70
1:B:354:ASP:HB3	1:B:357:LYS:HB2	1.75	0.69
1:A:9:CYS:SG	1:A:68:LYS:HE2	2.34	0.67
1:B:373:ASP:O	1:B:375:THR:N	2.26	0.67
1:B:195:CYS:SG	1:B:279:LEU:HD11	2.36	0.66
1:B:154:GLY:O	1:B:274:VAL:HG11	1.95	0.66
1:A:393:ARG:HH11	1:A:393:ARG:CG	2.09	0.65
1:A:325:THR:HG21	1:A:332:ILE:HD11	1.79	0.63
1:A:486:ARG:HG2	1:A:486:ARG:NH1	2.14	0.63
1:A:431:ILE:HD13	1:A:431:ILE:O	1.98	0.62
1:A:332:ILE:HD13	1:A:351:ILE:HD13	1.80	0.62
1:A:9:CYS:SG	1:A:68:LYS:CE	2.87	0.62
1:A:61:GLN:HG2	1:A:64:ARG:NH1	2.15	0.62
1:A:241:ALA:HA	1:A:379:LEU:HD21	1.82	0.61
1:B:231:ARG:HA	1:B:234:ARG:HH12	1.65	0.61
1:B:238:HIS:ND1	1:B:348:SER:HB3	2.14	0.61
1:A:247:ASP:OD2	1:A:300:SER:HB3	2.01	0.60
1:B:431:ILE:O	1:B:433:HIS:N	2.33	0.60
1:B:17:GLY:HA3	1:B:288:GLY:O	2.01	0.59
1:B:61:GLN:HE21	1:B:64:ARG:HD2	1.67	0.59
1:B:240:ASP:H	1:B:371:ARG:HH12	1.51	0.58
1:B:245:ARG:HH21	1:B:368:LYS:HE3	1.69	0.58
1:A:214:PRO:HB3	1:A:338:PHE:HB2	1.87	0.57
1:B:442:SER:HB2	1:B:503:PHE:CZ	2.40	0.56
1:A:486:ARG:HH11	1:A:486:ARG:CG	2.17	0.55
1:A:61:GLN:HG2	1:A:64:ARG:HH12	1.71	0.55
1:B:485:MET:HE3	1:B:485:MET:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ARG:CG	1:B:372:PRO:HD2	2.37	0.54
1:A:72:GLU:HG3	1:A:73:PRO:HD2	1.90	0.54
1:A:200:GLY:HA2	1:A:203:MET:HE2	1.90	0.53
1:B:321:LEU:HD22	1:B:353:LEU:HD22	1.92	0.52
1:B:190:ALA:O	1:B:194:ARG:HG3	2.09	0.52
1:B:496:ASP:HB3	1:B:499:LEU:HG	1.90	0.52
1:A:346:ILE:CD1	1:A:390:PHE:HB2	2.39	0.52
1:B:61:GLN:HG2	1:B:64:ARG:NH1	2.25	0.52
1:B:105:SER:OG	1:B:108:GLN:HG3	2.10	0.52
1:B:187:SER:HB3	1:B:192:MET:HE3	1.91	0.52
1:B:234:ARG:HB2	1:B:234:ARG:HH11	1.74	0.51
1:A:217:VAL:HA	1:A:341:TYR:CE2	2.45	0.51
1:A:452:PRO:HA	1:A:478:GLN:HG3	1.91	0.51
1:A:43:PRO:HG2	1:A:426:PRO:HB3	1.94	0.50
1:B:423:HIS:CE1	1:B:425:ASP:O	2.65	0.50
1:B:246:TRP:CG	1:B:343:ASP:HB3	2.47	0.50
1:A:354:ASP:HB3	1:A:357:LYS:HB2	1.93	0.50
1:A:221:MET:HE3	1:A:393:ARG:HG3	1.94	0.49
1:B:98:ILE:HG22	1:B:209:HIS:CD2	2.46	0.49
1:A:393:ARG:CG	1:A:393:ARG:NH1	2.70	0.49
1:B:482:PHE:CZ	1:B:486:ARG:HG3	2.48	0.49
1:B:325:THR:HB	1:B:327:LEU:HD12	1.95	0.49
1:A:14:LEU:HD11	1:A:293:SER:HB2	1.95	0.48
1:B:309:ASN:HB3	1:B:342:GLY:HA2	1.94	0.48
1:A:174:LYS:HG2	1:A:180:LYS:HB2	1.95	0.48
1:B:174:LYS:HD2	1:B:180:LYS:HB2	1.96	0.48
1:B:221:MET:HE3	1:B:404:GLY:HA3	1.95	0.48
1:B:393:ARG:HG3	1:B:406:LEU:HA	1.96	0.48
1:A:445:GLY:CA	1:A:485:MET:HE3	2.43	0.48
1:A:313:HIS:CE1	1:A:345:GLU:HB3	2.49	0.47
1:B:302:VAL:O	1:B:304:CYS:N	2.46	0.47
1:A:43:PRO:HD3	1:A:417:TRP:CZ2	2.49	0.47
1:A:41:TYR:HB2	1:A:413:ARG:HD3	1.96	0.47
1:A:485:MET:HE1	1:A:501:PRO:HG2	1.97	0.47
1:A:123:HIS:CE1	1:A:139:LYS:HB3	2.50	0.46
1:B:415:MET:HE2	1:B:461:LEU:HB2	1.98	0.46
1:A:153:GLU:H	1:A:153:GLU:HG2	1.47	0.46
1:A:393:ARG:HG2	1:A:393:ARG:NH1	2.16	0.46
1:A:242:ASP:O	1:A:370:THR:HB	2.15	0.46
1:B:63:MET:HG3	1:B:183:LEU:HD13	1.97	0.46
1:B:74:ARG:HB3	1:B:251:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ARG:O	1:B:406:LEU:HD12	2.16	0.45
1:B:126:ARG:HH11	1:B:126:ARG:HG2	1.81	0.45
1:B:203:MET:SD	1:B:307:GLN:HG2	2.57	0.45
1:B:126:ARG:O	1:B:126:ARG:HG3	2.12	0.45
1:A:130:CYS:C	1:A:137:THR:HB	2.42	0.44
1:A:121:HIS:HA	1:A:122:PRO:HA	1.68	0.44
1:B:305:THR:O	1:B:309:ASN:HB2	2.18	0.44
1:A:216:ARG:HE	1:A:339:SER:HA	1.83	0.44
1:A:321:LEU:O	1:A:325:THR:HB	2.17	0.44
1:A:182:ARG:HB2	1:A:182:ARG:HH11	1.82	0.44
1:B:216:ARG:CZ	1:B:228:ILE:HG12	2.48	0.44
1:A:246:TRP:CE2	1:A:250:GLN:NE2	2.85	0.44
1:B:405:LYS:HE3	1:B:450:HIS:CE1	2.53	0.44
1:B:76:LYS:HA	1:B:77:PRO:HD3	1.91	0.44
1:A:440:LEU:HD13	1:A:462:VAL:HG13	2.00	0.44
1:B:388:LEU:HD23	1:B:388:LEU:HA	1.90	0.43
1:B:432:PRO:O	1:B:433:HIS:C	2.61	0.43
1:A:341:TYR:CG	1:A:391:LEU:HD21	2.53	0.43
1:A:45:TYR:OH	1:A:57:PRO:O	2.27	0.43
1:A:63:MET:HE1	1:A:163:GLY:C	2.44	0.43
1:B:228:ILE:HG22	1:B:229:PHE:N	2.33	0.43
1:A:385:LEU:HG	1:A:395:VAL:HG21	2.01	0.43
1:A:431:ILE:HD13	1:A:431:ILE:C	2.44	0.43
1:A:341:TYR:CD2	1:A:391:LEU:HD21	2.54	0.42
1:B:241:ALA:O	1:B:242:ASP:C	2.63	0.42
1:A:221:MET:HG2	1:A:393:ARG:HG3	2.01	0.42
1:A:339:SER:O	1:A:345:GLU:HA	2.19	0.42
1:A:484:TRP:CD1	1:A:501:PRO:HD2	2.54	0.42
1:A:37:PRO:HA	1:A:38:PRO:HD3	1.92	0.42
1:B:234:ARG:HB2	1:B:234:ARG:NH1	2.34	0.42
1:B:441:MET:HE2	1:B:473:PHE:CZ	2.55	0.42
1:A:219:MET:HE2	1:A:221:MET:HA	2.01	0.42
1:A:302:VAL:HB	1:A:305:THR:CG2	2.50	0.42
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.89	0.41
1:B:409:SER:O	1:B:412:LEU:HG	2.20	0.41
1:B:458:ILE:HA	1:B:461:LEU:HD12	2.02	0.41
1:A:100:PRO:HA	1:A:101:PRO:HD3	1.91	0.41
1:A:26:THR:HB	1:A:46:LEU:HD21	2.03	0.41
1:A:346:ILE:HD12	1:A:390:PHE:HB2	2.02	0.41
1:B:281:SER:O	1:B:282:PRO:C	2.63	0.41
1:B:241:ALA:CA	1:B:379:LEU:HD21	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ALA:HA	1:B:280:LEU:HD11	2.03	0.41
1:A:391:LEU:O	1:A:393:ARG:NH1	2.54	0.41
1:B:313:HIS:CE1	1:B:345:GLU:HB3	2.56	0.41
1:B:30:ARG:HG2	1:B:417:TRP:CZ3	2.56	0.41
1:A:398:ASP:HB2	1:A:399:PRO:HD2	2.02	0.40
1:A:479:GLU:HB2	1:A:480:PRO:HD3	2.03	0.40
1:B:477:ARG:C	1:B:480:PRO:HD2	2.45	0.40
1:A:445:GLY:HA3	1:A:485:MET:HE3	2.02	0.40
1:A:114:ASP:O	1:A:127:LYS:HE2	2.21	0.40
1:A:199:PHE:O	1:A:200:GLY:C	2.64	0.40
1:B:221:MET:HE2	1:B:393:ARG:CB	2.51	0.40
1:B:346:ILE:HD11	1:B:390:PHE:HB2	2.02	0.40
1:A:113:LEU:HD22	1:A:192:MET:HB3	2.03	0.40
1:B:61:GLN:O	1:B:64:ARG:HB2	2.21	0.40
1:B:185:TRP:CD1	1:B:185:TRP:N	2.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	500/510 (98%)	470 (94%)	25 (5%)	5 (1%)	12	32
1	B	501/510 (98%)	453 (90%)	38 (8%)	10 (2%)	6	16
All	All	1001/1020 (98%)	923 (92%)	63 (6%)	15 (2%)	8	23

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	303	PRO
1	B	374	LYS
1	B	432	PRO

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Mol	Chain	Res	Type
1	B	434	SER
1	A	505	ASN
1	B	155	LYS
1	B	242	ASP
1	B	433	HIS
1	A	433	HIS
1	B	137	THR
1	A	242	ASP
1	B	302	VAL
1	A	504	VAL
1	A	399	PRO
1	B	399	PRO

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	433/438 (99%)	371 (86%)	62 (14%)	3	9
1	B	434/438 (99%)	353 (81%)	81 (19%)	1	4
All	All	867/876 (99%)	724 (84%)	143 (16%)	2	7

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	21	LYS
1	A	22	LEU
1	A	27	LYS
1	A	54	LYS
1	A	61	GLN
1	A	72	GLU
1	A	81	SER
1	A	82	VAL
1	A	89	THR
1	A	95	GLU

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Mol	Chain	Res	Type
1	A	112	SER
1	A	127	LYS
1	A	134	GLU
1	A	135	SER
1	A	137	THR
1	A	140	LEU
1	A	145	SER
1	A	146	LYS
1	A	149	LEU
1	A	153	GLU
1	A	155	LYS
1	A	171	LYS
1	A	172	THR
1	A	179	ILE
1	A	182	ARG
1	A	193	ILE
1	A	195	CYS
1	A	203	MET
1	A	211	VAL
1	A	285	VAL
1	A	289	ASP
1	A	298	LEU
1	A	306	SER
1	A	325	THR
1	A	346	ILE
1	A	356	GLU
1	A	357	LYS
1	A	375	THR
1	A	376	GLU
1	A	388	LEU
1	A	389	THR
1	A	392	ARG
1	A	393	ARG
1	A	395	VAL
1	A	396	THR
1	A	397	ARG
1	A	405	LYS
1	A	430	MET
1	A	431	ILE
1	A	439	GLN
1	A	460	LYS
1	A	467	LYS

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Mol	Chain	Res	Type
1	A	468	GLU
1	A	471	MET
1	A	472	ASP
1	A	483	ARG
1	A	486	ARG
1	A	499	LEU
1	A	502	SER
1	A	504	VAL
1	A	506	GLU
1	B	18	SER
1	B	21	LYS
1	B	24	THR
1	B	25	LYS
1	B	30	ARG
1	B	36	LEU
1	B	54	LYS
1	B	58	SER
1	B	61	GLN
1	B	68	LYS
1	B	82	VAL
1	B	95	GLU
1	B	98	ILE
1	B	99	ASP
1	B	112	SER
1	B	115	LYS
1	B	125	MET
1	B	126	ARG
1	B	146	LYS
1	B	149	LEU
1	B	155	LYS
1	B	158	THR
1	B	172	THR
1	B	174	LYS
1	B	182	ARG
1	B	193	ILE
1	B	195	CYS
1	B	203	MET
1	B	211	VAL
1	B	231	ARG
1	B	234	ARG
1	B	238	HIS
1	B	242	ASP

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Mol	Chain	Res	Type
1	B	254	VAL
1	B	260	GLU
1	B	262	MET
1	B	267	SER
1	B	277	GLU
1	B	295	ASN
1	B	298	LEU
1	B	322	SER
1	B	330	ASP
1	B	337	LEU
1	B	348	SER
1	B	351	ILE
1	B	352	LYS
1	B	353	LEU
1	B	357	LYS
1	B	359	THR
1	B	361	LYS
1	B	367	LEU
1	B	368	LYS
1	B	370	THR
1	B	371	ARG
1	B	374	LYS
1	B	375	THR
1	B	376	GLU
1	B	379	LEU
1	B	380	VAL
1	B	381	ILE
1	B	389	THR
1	B	392	ARG
1	B	393	ARG
1	B	410	SER
1	B	429	THR
1	B	433	HIS
1	B	438	ILE
1	B	444	LEU
1	B	457	LYS
1	B	460	LYS
1	B	461	LEU
1	B	466	LEU
1	B	467	LYS
1	B	474	TYR
1	B	478	GLN

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Mol	Chain	Res	Type
1	B	479	GLU
1	B	483	ARG
1	B	485	MET
1	B	502	SER
1	B	504	VAL
1	B	506	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	121	HIS
1	A	273	GLN
1	B	61	GLN
1	B	92	ASN
1	B	123	HIS
1	B	209	HIS
1	B	295	ASN
1	B	422	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	502/510 (98%)	-0.56	0	100 100	3, 17, 30, 51	0
1	B	503/510 (98%)	0.13	4 (0%)	82 78	2, 17, 29, 53	0
All	All	1005/1020 (98%)	-0.22	4 (0%)	88 86	2, 17, 29, 53	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	3.3
1	B	433	HIS	3.2
1	B	378	PRO	2.2
1	B	137	THR	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	600	1/1	0.85	0.13	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	600	1/1	0.88	0.32	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.