



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:22 PM UTC

PDB ID : 2JDQ / pdb_00002jdg
Title : C-terminal domain of influenza A virus polymerase PB2 subunit in complex with human importin alpha5
Authors : Tarendeau, F.; Guigay, D.; Mas, P.; Boulo, S.; Baudin, F.; Ruigrok, R.W.H.; Hart, D.J.; Cusack, S.
Deposited on : 2007-01-11
Resolution : 2.20 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

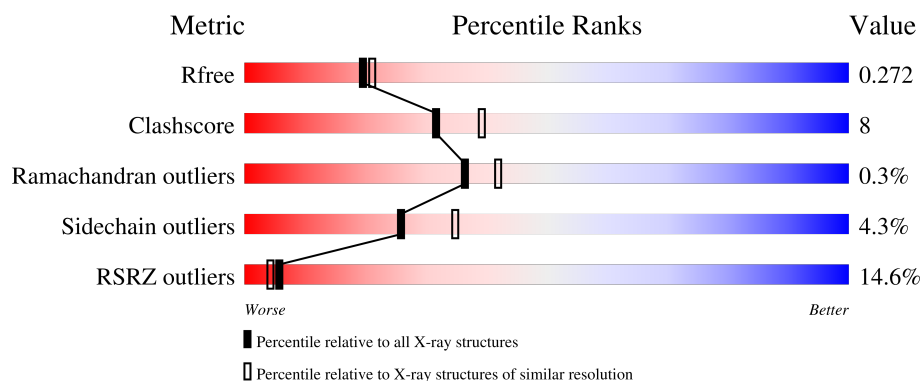
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	450	7% 79% 14% 6%
1	B	450	21% 78% 14% 5%
2	D	83	10% 66% 8% 24%
2	E	83	12% 58% 16% 5% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7862 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 IMPORTIN ALPHA-1 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3296	2094	554	630	18			
1	B	426	Total	C	N	O	S	0	0	0
			3313	2103	556	636	18			

- Molecule 2 is a protein called POLYMERASE BASIC PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	63	Total	C	N	O	S	0	0	0
			488	304	95	87	2			
2	E	65	Total	C	N	O	S	0	0	0
			500	312	96	90	2			

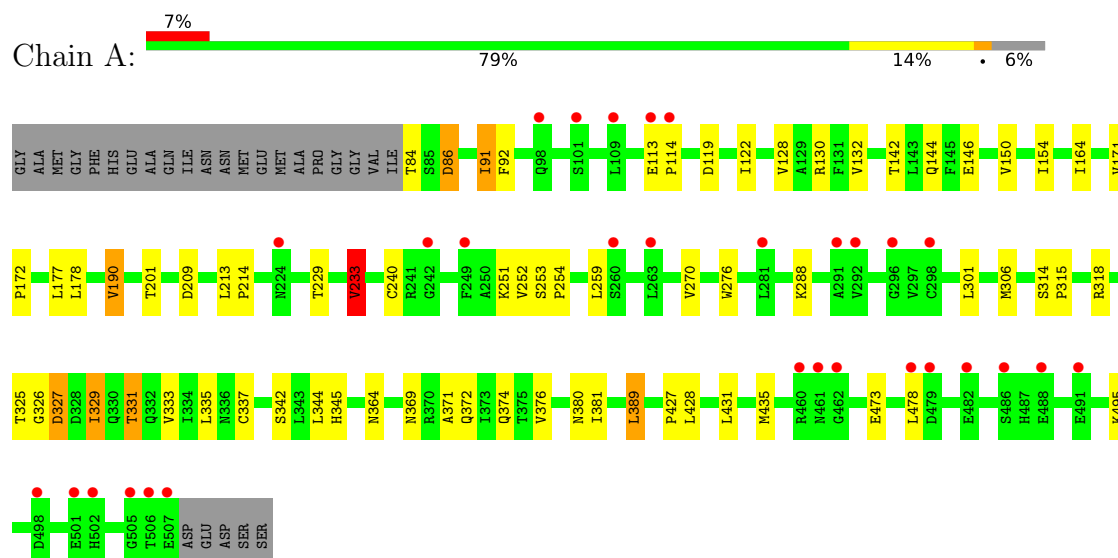
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	98	Total	O	0	0
			98	98		
3	D	14	Total	O	0	0
			14	14		
3	E	22	Total	O	0	0
			22	22		

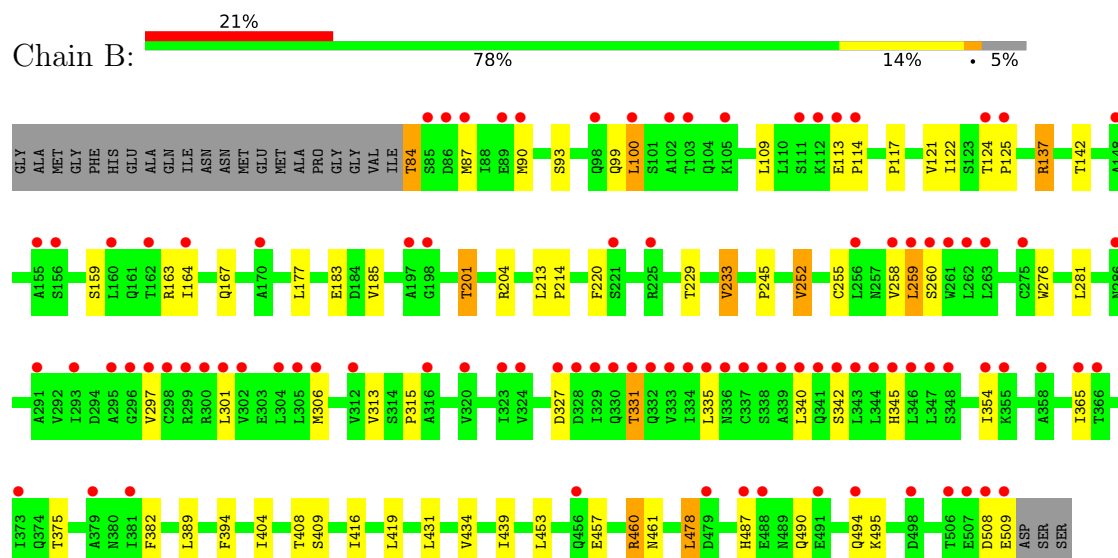
3 Residue-property plots [i](#)

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: IMPORTIN ALPHA-1 SUBUNIT

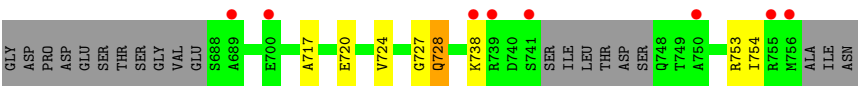


• Molecule 1: IMPORTIN ALPHA-1 SUBUNIT



• Molecule 2: POLYMERASE BASIC PROTEIN 2





● Molecule 2: POLYMERASE BASIC PROTEIN 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.97Å 100.55Å 151.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 30.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-2.20) 99.5 (30.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.247 0.242 , 0.272	Depositor DCC
R_{free} test set	2970 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7862	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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](#)

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	0.82	3/3354 (0.1%)	0.97	3/4558 (0.1%)
1	B	0.72	0/3371	0.88	1/4581 (0.0%)
2	D	0.57	0/489	0.75	0/649
2	E	0.62	0/501	0.73	0/666
All	All	0.75	3/7715 (0.0%)	0.91	4/10454 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	333	VAL	C-O	-7.09	1.15	1.24
1	A	329	ILE	CA-CB	6.35	1.62	1.54
1	A	374	GLN	N-CA	5.27	1.52	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	CYS	N-CA-C	-8.57	101.83	112.88
1	B	394	PHE	N-CA-C	5.60	117.39	111.28
1	A	233	VAL	CB-CA-C	-5.42	104.75	112.22
1	A	333	VAL	CB-CA-C	-5.01	105.47	112.04

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	3296	0	3331	46	0
1	B	3313	0	3341	61	0
2	D	488	0	528	5	0
2	E	500	0	540	20	0
3	A	131	0	0	4	0
3	B	98	0	0	1	0
3	D	14	0	0	0	0
3	E	22	0	0	5	0
All	All	7862	0	7740	124	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 (124) 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)
2:E:691:LEU:HD11	2:E:726:ILE:HD12	1.46	0.97
1:A:122:ILE:HG21	1:A:164:ILE:HD13	1.48	0.92
2:E:694:PHE:O	3:E:2007:HOH:O	1.90	0.88
1:B:306:MET:HA	1:B:306:MET:HE2	1.57	0.86
1:B:201:THR:HG21	1:B:245:PRO:HD2	1.55	0.86
1:B:100:LEU:HD21	1:B:142:THR:HG22	1.59	0.85
1:B:340:LEU:HD12	1:B:375:THR:HG22	1.60	0.83
1:B:122:ILE:HG21	1:B:164:ILE:HD13	1.60	0.83
1:A:229:THR:O	1:A:233:VAL:HG23	1.81	0.81
2:E:694:PHE:C	3:E:2007:HOH:O	2.26	0.79
1:A:389:LEU:HD13	1:A:427:PRO:HB2	1.65	0.77
1:B:461:ASN:HB3	3:B:2085:HOH:O	1.84	0.77
1:A:209:ASP:OD1	1:A:251:LYS:NZ	2.13	0.76
1:A:122:ILE:HD11	1:A:154:ILE:HG23	1.68	0.75
1:B:331:THR:HG21	2:D:738:LYS:NZ	2.02	0.75
1:B:122:ILE:CG2	1:B:164:ILE:HD13	2.17	0.74
1:A:122:ILE:CG2	1:A:164:ILE:HD13	2.19	0.73
1:B:306:MET:HE1	1:B:345:HIS:CD2	2.24	0.72
1:B:229:THR:O	1:B:233:VAL:HG23	1.91	0.71
1:B:327:ASP:O	1:B:331:THR:HG23	1.90	0.71
1:B:416:ILE:HG12	1:B:453:LEU:HD12	1.74	0.69
1:A:473:GLU:OE2	1:A:478:LEU:HD13	1.93	0.68
2:E:713:LEU:HD13	2:E:724:VAL:CG1	2.24	0.67
1:B:306:MET:HE1	1:B:345:HIS:HD2	1.60	0.67
1:A:327:ASP:O	1:A:331:THR:HG23	1.94	0.66
2:E:696:ILE:HG23	2:E:732:VAL:CG1	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:713:LEU:HD13	2:E:724:VAL:HG13	1.78	0.66
2:E:696:ILE:HG23	2:E:732:VAL:HG13	1.77	0.66
1:B:434:VAL:HG21	1:B:439:ILE:HG21	1.77	0.65
1:B:431:LEU:O	1:B:434:VAL:HG22	1.98	0.64
1:A:306:MET:HE1	1:A:345:HIS:CD2	2.32	0.63
1:B:340:LEU:CD1	1:B:375:THR:HG22	2.28	0.63
1:A:306:MET:HE1	1:A:345:HIS:HD2	1.64	0.63
1:B:389:LEU:HD11	1:B:431:LEU:HD11	1.83	0.61
1:B:331:THR:HG21	2:D:738:LYS:HZ2	1.65	0.60
2:E:737:ARG:NE	3:E:2007:HOH:O	2.35	0.58
1:B:408:THR:HA	1:B:416:ILE:HD11	1.85	0.58
1:A:84:THR:HG22	1:A:86:ASP:H	1.69	0.58
1:B:460:ARG:HH12	1:B:461:ASN:HB2	1.69	0.57
1:A:240:CYS:SG	1:A:252:VAL:CG1	2.93	0.57
1:B:201:THR:HG23	1:B:204:ARG:NH2	2.20	0.57
1:B:404:ILE:O	1:B:408:THR:HG23	2.04	0.56
1:A:233:VAL:HG21	1:A:270:VAL:HG13	1.86	0.56
1:B:508:ASP:O	1:B:509:GLU:HB2	2.06	0.56
1:B:382:PHE:CD2	1:B:419:LEU:HD21	2.40	0.56
1:B:416:ILE:HG12	1:B:453:LEU:CD1	2.36	0.55
1:A:344:LEU:HB2	1:A:381:ILE:HD13	1.88	0.54
1:B:335:LEU:HD21	1:B:365:ILE:HD13	1.90	0.54
1:B:117:PRO:O	1:B:121:VAL:HG23	2.08	0.53
1:B:306:MET:HE3	1:B:342:SER:HB3	1.91	0.53
2:E:686:VAL:HG23	2:E:687:GLU:H	1.74	0.52
1:B:201:THR:HG21	1:B:245:PRO:CD	2.35	0.51
1:A:91:ILE:HG23	1:A:130:ARG:HG2	1.92	0.51
1:A:318:ARG:NE	3:A:2054:HOH:O	2.42	0.51
1:A:329:ILE:CD1	1:B:478:LEU:HD21	2.40	0.51
1:B:260:SER:HA	1:B:297:VAL:HG12	1.93	0.50
1:A:331:THR:HG21	2:E:738:LYS:NZ	2.27	0.50
1:B:100:LEU:HD11	1:B:142:THR:CG2	2.42	0.49
1:A:329:ILE:HD11	1:B:478:LEU:HD21	1.94	0.49
1:A:335:LEU:HD12	1:A:372:GLN:HG2	1.95	0.49
1:A:171:VAL:HB	1:A:172:PRO:HD3	1.94	0.48
1:B:122:ILE:HD13	1:B:164:ILE:CD1	2.43	0.48
1:A:318:ARG:HD3	3:A:2054:HOH:O	2.14	0.48
1:A:327:ASP:O	1:A:331:THR:CG2	2.61	0.48
1:A:318:ARG:CD	3:A:2054:HOH:O	2.62	0.47
2:E:725:LEU:HD12	2:E:731:VAL:HG22	1.97	0.47
1:B:508:ASP:O	1:B:509:GLU:CB	2.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ILE:HD13	1:B:164:ILE:HD13	1.97	0.47
1:B:177:LEU:HD22	1:B:185:VAL:HG11	1.97	0.46
1:B:109:LEU:HD22	1:B:117:PRO:HG3	1.97	0.46
1:A:288:LYS:HD3	3:A:2038:HOH:O	2.16	0.46
1:A:325:THR:HG22	1:A:364:ASN:ND2	2.31	0.46
1:B:340:LEU:HD12	1:B:375:THR:CG2	2.39	0.46
1:B:434:VAL:CG2	1:B:439:ILE:HG21	2.44	0.46
1:A:213:LEU:HB3	1:A:214:PRO:HD3	1.98	0.45
2:D:727:GLY:O	2:D:728:GLN:C	2.59	0.45
1:B:331:THR:HG21	2:D:738:LYS:HZ1	1.77	0.45
2:E:713:LEU:HD13	2:E:724:VAL:HG11	1.95	0.45
1:B:124:THR:HG23	1:B:125:PRO:HD2	1.98	0.45
1:A:473:GLU:OE2	1:A:478:LEU:CD1	2.64	0.45
1:B:100:LEU:HD11	1:B:142:THR:HB	1.98	0.45
1:A:91:ILE:HG22	1:A:92:PHE:N	2.31	0.45
1:B:113:GLU:N	1:B:114:PRO:HD2	2.32	0.45
1:B:252:VAL:HG13	1:B:281:LEU:HD21	1.99	0.45
2:E:737:ARG:CZ	3:E:2007:HOH:O	2.63	0.45
1:B:213:LEU:HB3	1:B:214:PRO:HD3	1.99	0.44
1:A:144:GLN:NE2	1:A:177:LEU:HD21	2.32	0.44
1:B:434:VAL:CG2	1:B:439:ILE:CG2	2.95	0.44
2:D:717:ALA:HB3	2:D:720:GLU:CG	2.47	0.44
1:A:128:VAL:O	1:A:132:VAL:HG23	2.18	0.44
1:A:253:SER:N	1:A:254:PRO:CD	2.81	0.44
2:E:727:GLY:O	2:E:728:GLN:C	2.60	0.43
1:B:276:TRP:CD2	1:B:315:PRO:HB3	2.53	0.43
1:A:178:LEU:CD2	1:A:190:VAL:HG23	2.47	0.43
1:A:146:GLU:O	1:A:150:VAL:HG23	2.18	0.43
1:B:163:ARG:HG2	1:B:167:GLN:HE21	1.84	0.43
1:A:326:GLY:C	1:A:327:ASP:O	2.58	0.43
1:B:90:MET:O	1:B:93:SER:OG	2.34	0.43
1:A:389:LEU:HD21	1:A:431:LEU:HD11	2.00	0.42
1:B:177:LEU:HD22	1:B:185:VAL:CG1	2.48	0.42
1:B:457:GLU:OE2	1:B:460:ARG:NH1	2.52	0.42
2:E:694:PHE:CZ	2:E:713:LEU:HG	2.54	0.42
1:B:487:HIS:HD2	1:B:490:GLN:HE21	1.65	0.42
2:E:713:LEU:HD22	2:E:724:VAL:HG11	2.00	0.42
1:A:306:MET:HE3	1:A:342:SER:HB3	2.00	0.42
1:A:376:VAL:HG13	1:A:381:ILE:HG13	2.01	0.42
1:A:240:CYS:SG	1:A:252:VAL:HG11	2.58	0.42
1:A:113:GLU:N	1:A:114:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:SER:HB2	1:A:315:PRO:CD	2.50	0.42
1:A:435:MET:HE3	1:A:435:MET:HA	2.03	0.41
1:B:84:THR:N	1:B:87:MET:SD	2.93	0.41
1:B:99:GLN:OE1	1:B:137:ARG:NH2	2.53	0.41
2:E:740:ASP:HB2	3:E:2022:HOH:O	2.20	0.41
1:B:93:SER:O	1:B:99:GLN:NE2	2.46	0.41
1:B:124:THR:CG2	1:B:125:PRO:HD2	2.51	0.41
1:B:220:PHE:CD1	1:B:258:VAL:HG11	2.56	0.41
1:A:369:ASN:OD1	1:A:369:ASN:C	2.64	0.41
1:B:460:ARG:NH1	1:B:461:ASN:HB2	2.35	0.41
2:E:691:LEU:CD1	2:E:726:ILE:HD12	2.33	0.41
1:A:369:ASN:OD1	1:A:371:ALA:HB3	2.21	0.40
1:A:276:TRP:NE1	2:E:749:THR:HG21	2.36	0.40
1:A:331:THR:HG21	2:E:738:LYS:HZ2	1.86	0.40
1:B:255:CYS:SG	1:B:259:LEU:HD22	2.62	0.40
1:B:313:VAL:CG1	1:B:354:ILE:HD13	2.51	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	422/450 (94%)	414 (98%)	7 (2%)	1 (0%)	43	51
1	B	424/450 (94%)	414 (98%)	10 (2%)	0	100	100
2	D	59/83 (71%)	57 (97%)	1 (2%)	1 (2%)	7	5
2	E	61/83 (74%)	60 (98%)	0	1 (2%)	7	6
All	All	966/1066 (91%)	945 (98%)	18 (2%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
2	E	728	GLN
2	D	728	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/387 (95%)	354 (96%)	14 (4%)	29	40
1	B	370/387 (96%)	354 (96%)	16 (4%)	26	35
2	D	52/69 (75%)	49 (94%)	3 (6%)	18	22
2	E	53/69 (77%)	50 (94%)	3 (6%)	18	23
All	All	843/912 (92%)	807 (96%)	36 (4%)	26	35

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	91	ILE
1	A	119	ASP
1	A	142	THR
1	A	190	VAL
1	A	201	THR
1	A	233	VAL
1	A	259	LEU
1	A	301	LEU
1	A	331	THR
1	A	380	ASN
1	A	389	LEU
1	A	428	LEU
1	A	495	LYS
1	B	84	THR
1	B	100	LEU
1	B	137	ARG
1	B	159	SER
1	B	183	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	201	THR
1	B	233	VAL
1	B	252	VAL
1	B	259	LEU
1	B	301	LEU
1	B	331	THR
1	B	409	SER
1	B	460	ARG
1	B	478	LEU
1	B	494	GLN
1	B	495	LYS
2	D	724	VAL
2	D	753	ARG
2	D	754	ILE
2	E	686	VAL
2	E	724	VAL
2	E	732	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	144	GLN
1	A	186	GLN
1	A	224	ASN
1	A	257	ASN
1	A	345	HIS
1	A	380	ASN
1	A	390	GLN
1	A	485	GLN
1	A	490	GLN
1	A	494	GLN
1	A	502	HIS
1	B	98	GLN
1	B	167	GLN
1	B	223	GLN
1	B	332	GLN
1	B	345	HIS
1	B	372	GLN
1	B	485	GLN
1	B	487	HIS
2	D	715	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	728	GLN
2	D	748	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	424/450 (94%)	0.46	30 (7%) 22 19	2, 23, 36, 44	0
1	B	426/450 (94%)	1.11	95 (22%) 2 1	2, 24, 41, 52	0
2	D	63/83 (75%)	0.95	8 (12%) 8 6	15, 22, 56, 62	0
2	E	65/83 (78%)	0.99	10 (15%) 5 4	8, 16, 40, 44	0
All	All	978/1066 (91%)	0.81	143 (14%) 6 4	2, 22, 40, 62	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	508	ASP	6.2
1	B	332	GLN	4.8
1	A	507	GLU	4.5
1	B	334	ILE	4.4
1	A	498	ASP	4.3
1	B	335	LEU	4.2
1	B	102	ALA	4.1
1	B	337	CYS	4.0
1	B	329	ILE	4.0
1	B	328	ASP	4.0
1	B	87	MET	3.9
1	B	347	LEU	3.9
1	B	286	ASN	3.8
2	D	741	SER	3.8
1	B	331	THR	3.8
1	B	338	SER	3.8
2	E	729	GLY	3.8
1	B	86	ASP	3.7
1	B	89	GLU	3.7
1	B	263	LEU	3.7
1	A	114	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	342	SER	3.7
2	E	741	SER	3.6
1	B	302	VAL	3.6
1	B	339	ALA	3.6
1	B	344	LEU	3.5
1	B	343	LEU	3.5
1	B	299	ARG	3.5
2	E	739	ARG	3.5
1	B	297	VAL	3.4
1	B	298	CYS	3.4
1	B	509	GLU	3.4
1	B	324	VAL	3.4
1	B	340	LEU	3.4
1	B	323	ILE	3.3
1	B	111	SER	3.3
1	B	293	ILE	3.3
1	B	113	GLU	3.3
1	B	112	LYS	3.3
1	B	198	GLY	3.2
1	A	461	ASN	3.2
1	B	304	LEU	3.2
1	B	320	VAL	3.2
1	B	333	VAL	3.2
2	E	689	ALA	3.2
1	B	330	GLN	3.2
1	B	291	ALA	3.1
1	B	301	LEU	3.1
1	B	114	PRO	3.1
1	B	341	GLN	3.0
1	B	316	ALA	3.0
1	B	306	MET	3.0
1	B	488	GLU	3.0
2	D	750	ALA	3.0
1	A	479	ASP	2.9
1	B	507	GLU	2.9
1	A	488	GLU	2.9
1	B	479	ASP	2.9
1	B	164	ILE	2.9
2	D	756	MET	2.8
1	B	354	ILE	2.8
1	B	225	ARG	2.8
1	B	98	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	259	LEU	2.8
1	A	506	THR	2.8
1	B	261	TRP	2.7
2	E	740	ASP	2.7
1	B	296	GLY	2.7
1	B	336	ASN	2.7
1	A	486	SER	2.7
2	D	738	LYS	2.7
1	B	295	ALA	2.7
1	B	300	ARG	2.7
1	B	494	GLN	2.6
2	E	687	GLU	2.6
2	E	711	ASN	2.6
1	A	291	ALA	2.6
1	B	103	THR	2.6
1	A	502	HIS	2.6
1	A	98	GLN	2.6
1	B	221	SER	2.6
1	B	148	ALA	2.6
1	B	124	THR	2.6
1	B	373	ILE	2.6
1	A	478	LEU	2.5
1	B	160	LEU	2.5
1	B	346	LEU	2.5
1	B	170	ALA	2.5
1	B	90	MET	2.5
2	D	689	ALA	2.5
1	A	281	LEU	2.5
1	B	256	LEU	2.5
2	E	695	LEU	2.5
1	A	296	GLY	2.5
1	B	456	GLN	2.5
1	B	381	ILE	2.4
1	A	224	ASN	2.4
1	B	487	HIS	2.4
1	A	491	GLU	2.4
1	B	262	LEU	2.4
1	B	345	HIS	2.4
2	D	739	ARG	2.4
1	A	260	SER	2.4
1	B	156	SER	2.4
1	B	100	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	305	LEU	2.4
1	A	482	GLU	2.4
1	A	505	GLY	2.3
1	B	348	SER	2.3
1	A	460	ARG	2.3
1	B	506	THR	2.3
1	B	312	VAL	2.3
1	B	275	CYS	2.3
2	D	755	ARG	2.3
2	E	737	ARG	2.3
1	B	327	ASP	2.2
1	B	197	ALA	2.2
1	B	491	GLU	2.2
2	D	700	GLU	2.2
1	B	365	ILE	2.2
1	B	366	THR	2.2
1	B	379	ALA	2.2
1	A	249	PHE	2.2
1	B	105	LYS	2.2
1	B	155	ALA	2.2
1	B	258	VAL	2.2
1	B	260	SER	2.2
1	B	162	THR	2.1
1	B	498	ASP	2.1
1	B	355	LYS	2.1
1	A	501	GLU	2.1
1	A	298	CYS	2.1
1	B	358	ALA	2.1
2	E	686	VAL	2.1
1	A	242	GLY	2.1
1	A	462	GLY	2.1
1	B	85	SER	2.0
1	A	263	LEU	2.0
1	B	125	PRO	2.0
1	A	292	VAL	2.0
1	A	101	SER	2.0
1	A	113	GLU	2.0
1	A	109	LEU	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 [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.