



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:12 AM UTC

PDB ID : 5TPN / pdb_00005tpn
Title : Crystal structure of RSV F in complex with human antibody hRSV90
Authors : Mousa, J.J.; Crowe, J.E.
Deposited on : 2016-10-20
Resolution : 3.14 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

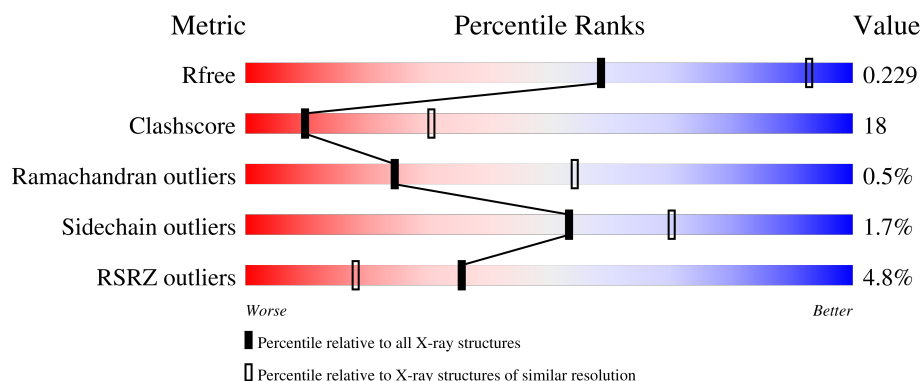
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	5% 68% 26% ..
2	H	225	4% 57% 37% ..
3	L	214	4% 62% 36% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7073 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 Fusion glycoprotein F0,Fibritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3783	2389	629	744	21			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	LYS	GLU	conflict	UNP P03420
A	67	ILE	ASN	engineered mutation	UNP P03420
A	76	ILE	VAL	conflict	UNP P03420
A	102	ALA	PRO	conflict	UNP P03420
A	128	GLN	ARG	conflict	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	GLU	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	PRO	deletion	UNP P03420
A	?	-	ARG	deletion	UNP P03420
A	?	-	PHE	deletion	UNP P03420
A	?	-	MET	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	TYR	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	ALA	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	LYS	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	ASN	deletion	UNP P03420
A	?	-	VAL	deletion	UNP P03420
A	?	-	THR	deletion	UNP P03420
A	?	-	LEU	deletion	UNP P03420
A	?	-	SER	deletion	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
A	131	GLY	LYS	linker	UNP P03420
A	132	SER	LYS	linker	UNP P03420
A	133	GLY	ARG	linker	UNP P03420
A	134	SER	LYS	linker	UNP P03420
A	135	GLY	ARG	linker	UNP P03420
A	137	SER	PHE	conflict	UNP P03420
A	215	PRO	SER	engineered mutation	UNP P03420
A	379	VAL	ILE	engineered mutation	UNP P03420
A	447	VAL	MET	engineered mutation	UNP P03420
A	487	GLN	GLU	conflict	UNP P03420
A	514	SER	-	linker	UNP P03420
A	515	ALA	-	linker	UNP P03420
A	516	ILE	-	linker	UNP P03420
A	517	GLY	-	linker	UNP P03420
A	545	GLY	-	expression tag	UNP Q38650
A	546	GLY	-	expression tag	UNP Q38650
A	547	LEU	-	expression tag	UNP Q38650
A	548	VAL	-	expression tag	UNP Q38650
A	549	PRO	-	expression tag	UNP Q38650
A	550	ARG	-	expression tag	UNP Q38650
A	551	GLY	-	expression tag	UNP Q38650
A	552	SER	-	expression tag	UNP Q38650
A	553	HIS	-	expression tag	UNP Q38650
A	554	HIS	-	expression tag	UNP Q38650
A	555	HIS	-	expression tag	UNP Q38650
A	556	HIS	-	expression tag	UNP Q38650
A	557	HIS	-	expression tag	UNP Q38650
A	558	HIS	-	expression tag	UNP Q38650

- Molecule 2 is a protein called hRSV90 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1655	1051	280	319	5			

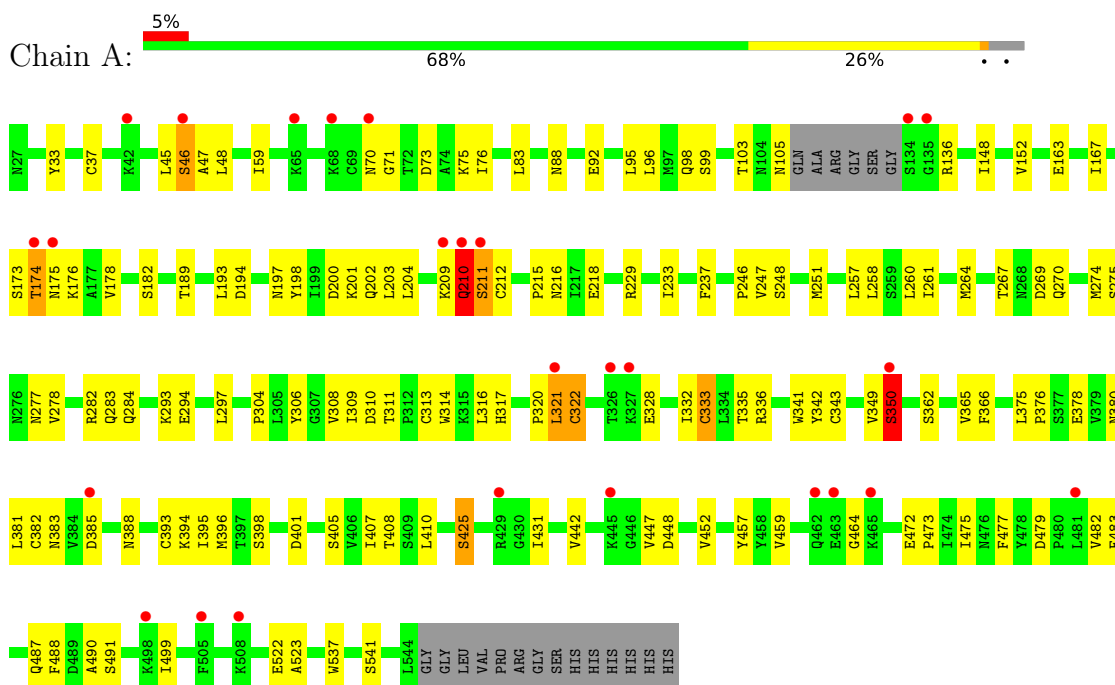
- Molecule 3 is a protein called hRSV0 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1635	1022	278	329	6			

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.

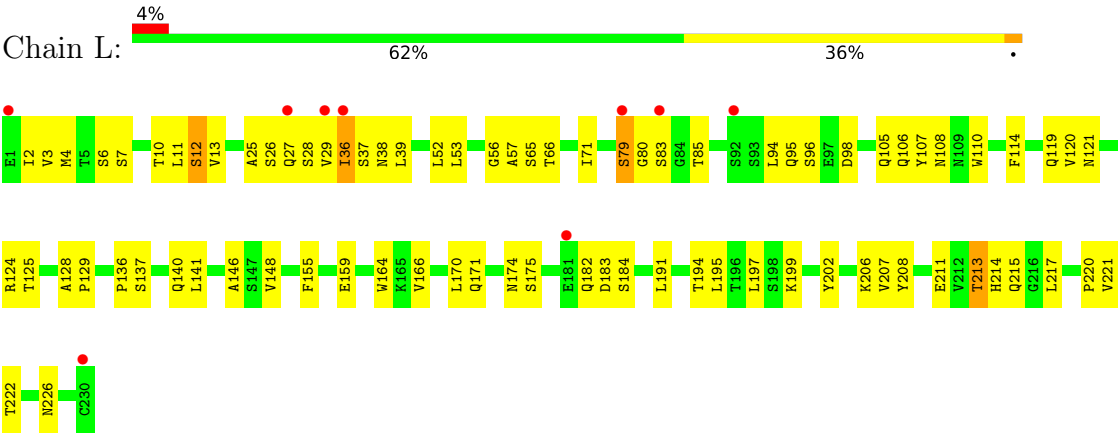
- Molecule 1: Fusion glycoprotein F0,Fibritin



- Molecule 2: hRSV90 heavy chain



- Molecule 3: hRSV0 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	148.25Å 148.25Å 538.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.29 – 3.14 49.29 – 3.14	Depositor EDS
% Data completeness (in resolution range)	75.7 (49.29-3.14) 75.7 (49.29-3.14)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 3.12Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.224 , 0.262 (Not available) , 0.229	Depositor DCC
R_{free} test set	1541 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7073	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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

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	0.51	0/3840	0.83	9/5205 (0.2%)
2	H	0.54	0/1697	0.89	3/2315 (0.1%)
3	L	0.59	0/1670	0.80	1/2270 (0.0%)
All	All	0.54	0/7207	0.84	13/9790 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	78	ILE	N-CA-C	12.94	126.52	107.37
1	A	210	GLN	N-CA-C	-11.67	90.81	109.59
1	A	46	SER	N-CA-C	9.87	125.07	108.20
2	H	57	THR	N-CA-C	9.30	127.29	107.67
1	A	321	LEU	N-CA-C	-7.53	99.31	110.46
3	L	80	GLY	N-CA-C	7.30	119.63	110.29
1	A	350	SER	N-CA-C	-6.39	101.53	110.35
1	A	70	ASN	CA-C-N	-5.95	112.56	121.01
1	A	70	ASN	C-N-CA	-5.95	112.56	121.01
1	A	382	CYS	CA-CB-SG	-5.79	101.08	114.40
1	A	71	GLY	N-CA-C	-5.51	104.07	112.51
2	H	78	ILE	CB-CA-C	-5.28	103.85	111.19
1	A	393	CYS	CA-CB-SG	-5.02	102.85	114.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3783	0	3835	106	0
2	H	1655	0	1607	81	0
3	L	1635	0	1576	72	0
All	All	7073	0	7018	248	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 18.

All (248) 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:46:SER:HB3	1:A:313:CYS:SG	1.70	1.29
2:H:76:PHE:CZ	2:H:91:MET:SD	2.37	1.18
3:L:29:VAL:HG11	3:L:106:GLN:HB2	1.21	1.10
1:A:178:VAL:CG2	3:L:36:ILE:HD11	1.91	1.01
3:L:29:VAL:HG11	3:L:106:GLN:CB	1.90	1.01
2:H:101:LEU:HG	2:H:122:THR:O	1.61	1.01
3:L:29:VAL:CG1	3:L:106:GLN:HB2	1.95	0.95
2:H:38:THR:CG2	2:H:57:THR:OG1	2.19	0.91
1:A:178:VAL:HG23	3:L:36:ILE:HD11	1.54	0.88
2:H:38:THR:HG21	2:H:57:THR:OG1	1.74	0.87
1:A:210:GLN:O	1:A:211:SER:C	2.14	0.87
2:H:41:TRP:HD1	2:H:78:ILE:HD12	1.39	0.87
2:H:59:ASN:O	2:H:62:SER:C	2.15	0.87
2:H:58:TRP:H	2:H:80:ARG:NH1	1.73	0.85
2:H:57:THR:O	2:H:58:TRP:HB3	1.74	0.84
1:A:178:VAL:HG21	3:L:36:ILE:HD11	1.59	0.82
1:A:174:THR:HG21	3:L:107:TYR:CD1	2.15	0.81
1:A:321:LEU:O	1:A:322:CYS:HB2	1.80	0.81
1:A:174:THR:HG21	3:L:107:TYR:HD1	1.46	0.81
3:L:13:VAL:HG23	3:L:94:LEU:HD12	1.64	0.77
2:H:201:SER:HA	2:H:204:LEU:HD13	1.67	0.75
2:H:76:PHE:CE1	2:H:91:MET:SD	2.80	0.75
2:H:168:SER:O	2:H:212:ASN:CB	2.35	0.74
1:A:174:THR:CG2	3:L:107:TYR:HD1	2.00	0.74
3:L:159:GLU:N	3:L:159:GLU:OE1	2.19	0.73
2:H:99:THR:HG22	2:H:126:VAL:H	1.53	0.73
2:H:91:MET:HE1	2:H:102:TYR:CZ	2.23	0.73
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.69	0.72
2:H:59:ASN:O	2:H:63:GLY:N	2.21	0.72
1:A:261:ILE:HG12	1:A:274:MET:HE3	1.72	0.72
3:L:214:HIS:CD2	3:L:215:GLN:H	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:168:SER:O	2:H:212:ASN:HB2	1.94	0.68
2:H:56:ILE:HD13	2:H:80:ARG:HD2	1.74	0.68
1:A:178:VAL:HG23	3:L:36:ILE:CD1	2.22	0.68
2:H:56:ILE:HG22	2:H:65:ILE:CG2	2.25	0.67
2:H:136:VAL:HG21	2:H:213:VAL:HG21	1.75	0.67
1:A:136:ARG:HH12	1:A:320:PRO:HG3	1.57	0.67
1:A:59:ILE:HG23	1:A:193:LEU:HB3	1.78	0.66
1:A:46:SER:HG	1:A:311:THR:HG1	1.44	0.65
1:A:267:THR:HG22	1:A:269:ASP:H	1.61	0.65
2:H:183:ALA:HA	2:H:193:LEU:HB3	1.78	0.65
2:H:56:ILE:HG22	2:H:65:ILE:HG22	1.77	0.64
2:H:76:PHE:HA	2:H:90:GLN:O	1.98	0.64
3:L:213:THR:HG22	3:L:220:PRO:HB3	1.79	0.64
2:H:78:ILE:HG23	2:H:78:ILE:O	1.96	0.64
2:H:58:TRP:H	2:H:80:ARG:HH12	1.46	0.63
2:H:13:VAL:HG21	2:H:19:LEU:HD22	1.80	0.63
3:L:129:PRO:HD2	3:L:217:LEU:HD21	1.78	0.63
1:A:46:SER:CB	1:A:313:CYS:SG	2.66	0.62
2:H:59:ASN:C	2:H:63:GLY:N	2.56	0.62
1:A:425:SER:HB3	1:A:431:ILE:HA	1.80	0.61
1:A:211:SER:N	1:A:212:CYS:HB3	2.15	0.61
3:L:174:ASN:OD1	3:L:174:ASN:N	2.33	0.61
1:A:173:SER:HB2	3:L:110:TRP:HE1	1.66	0.61
1:A:267:THR:HB	1:A:270:GLN:H	1.66	0.61
1:A:200:ASP:HA	1:A:204:LEU:HG	1.84	0.60
1:A:336:ARG:HA	1:A:395:ILE:HG22	1.83	0.60
2:H:94:LEU:HG	2:H:126:VAL:HG21	1.83	0.60
2:H:168:SER:O	2:H:212:ASN:HB3	2.01	0.60
1:A:229:ARG:O	1:A:233:ILE:HG13	2.02	0.59
3:L:207:VAL:HG22	3:L:226:ASN:OD1	2.03	0.59
2:H:38:THR:HG22	2:H:57:THR:OG1	2.02	0.59
1:A:248:SER:HB2	1:A:251:MET:H	1.68	0.59
1:A:321:LEU:O	1:A:322:CYS:CB	2.45	0.59
3:L:129:PRO:HD3	3:L:214:HIS:ND1	2.18	0.58
3:L:95:GLN:HG2	3:L:96:SER:H	1.67	0.58
2:H:99:THR:CG2	2:H:126:VAL:H	2.16	0.58
2:H:42:VAL:O	2:H:103:TYR:HB2	2.03	0.58
2:H:99:THR:HB	2:H:125:THR:HA	1.84	0.58
1:A:198:TYR:CE1	1:A:202:GLN:HG3	2.39	0.58
2:H:67:TYR:HE2	2:H:78:ILE:HG22	1.69	0.57
1:A:264:MET:SD	1:A:274:MET:HE1	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:LEU:HD11	1:A:336:ARG:NH2	2.19	0.57
3:L:3:VAL:H	3:L:26:SER:HB3	1.70	0.57
1:A:380:ASN:O	1:A:380:ASN:ND2	2.26	0.56
2:H:41:TRP:CD1	2:H:78:ILE:HD12	2.30	0.56
1:A:173:SER:O	1:A:174:THR:HB	2.06	0.55
3:L:183:ASP:OD1	3:L:184:SER:N	2.39	0.55
2:H:23:CYS:HB3	2:H:87:LEU:HB3	1.88	0.55
2:H:41:TRP:HD1	2:H:78:ILE:CD1	2.16	0.55
1:A:167:ILE:HG23	1:A:189:THR:HG21	1.88	0.55
2:H:81:ASP:C	2:H:83:ALA:H	2.14	0.55
2:H:180:THR:HG22	2:H:195:SER:OG	2.06	0.55
2:H:156:LEU:HD22	2:H:158:LYS:HB2	1.88	0.55
1:A:385:ASP:HB2	1:A:388:ASN:HB2	1.88	0.55
1:A:198:TYR:O	1:A:202:GLN:HB2	2.06	0.55
1:A:320:PRO:HA	1:A:335:THR:OG1	2.06	0.54
2:H:106:ARG:NH1	2:H:116:ASP:OD2	2.40	0.54
2:H:75:ARG:NH1	2:H:98:ASP:OD2	2.41	0.54
2:H:67:TYR:OH	2:H:77:THR:HA	2.08	0.54
2:H:76:PHE:CE2	2:H:91:MET:SD	2.99	0.54
1:A:136:ARG:NH1	1:A:320:PRO:HG3	2.21	0.54
2:H:17:ARG:HG2	2:H:18:SER:H	1.72	0.54
3:L:57:ALA:HB1	3:L:79:SER:O	2.08	0.54
3:L:29:VAL:CG1	3:L:106:GLN:CB	2.69	0.53
1:A:316:LEU:HD11	1:A:336:ARG:HH22	1.74	0.53
2:H:141:PRO:HD3	2:H:153:LEU:HB3	1.91	0.53
3:L:128:ALA:HB1	3:L:217:LEU:HD23	1.91	0.53
1:A:194:ASP:O	1:A:197:ASN:N	2.38	0.53
1:A:322:CYS:SG	1:A:401:ASP:HB3	2.48	0.53
2:H:35:ASP:O	2:H:58:TRP:HE3	1.91	0.53
1:A:257:LEU:HD22	1:A:278:VAL:HG13	1.90	0.53
3:L:10:THR:HG23	3:L:119:GLN:HB3	1.90	0.53
1:A:148:ILE:O	1:A:152:VAL:HG23	2.09	0.52
1:A:332:ILE:HB	1:A:483:PHE:CE2	2.45	0.52
3:L:174:ASN:CG	3:L:195:LEU:HD11	2.35	0.52
1:A:448:ASP:O	1:A:459:VAL:HG22	2.09	0.52
1:A:163:GLU:OE2	1:A:182:SER:N	2.42	0.52
3:L:121:ASN:HB2	3:L:182:GLN:OE1	2.10	0.52
2:H:6:GLU:CD	2:H:121:GLY:HA2	2.35	0.51
3:L:174:ASN:ND2	3:L:195:LEU:HD11	2.24	0.51
1:A:410:LEU:HD21	1:A:464:GLY:HA3	1.93	0.51
1:A:45:LEU:HD22	1:A:310:ASP:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:GLU:HG2	2:H:164:PRO:HA	1.92	0.51
2:H:56:ILE:HG23	2:H:78:ILE:HG23	1.93	0.51
1:A:522:GLU:HG3	1:A:523:ALA:O	2.10	0.51
1:A:308:VAL:O	1:A:309:ILE:HD13	2.11	0.50
1:A:209:LYS:HE2	1:A:212:CYS:H	1.77	0.50
1:A:201:LYS:HG3	2:H:58:TRP:CH2	2.47	0.50
1:A:96:LEU:HD13	1:A:237:PHE:HB3	1.94	0.49
1:A:163:GLU:OE2	1:A:182:SER:OG	2.21	0.49
3:L:206:LYS:HE3	3:L:226:ASN:HD22	1.78	0.49
2:H:87:LEU:HD12	2:H:88:TYR:H	1.76	0.49
2:H:163:GLU:HB2	2:H:191:TYR:CE2	2.48	0.49
3:L:105:GLN:HG2	3:L:106:GLN:N	2.27	0.49
3:L:175:SER:HA	3:L:194:THR:O	2.13	0.49
1:A:306:TYR:HB3	1:A:309:ILE:HD11	1.95	0.49
2:H:101:LEU:HD21	2:H:121:GLY:HA3	1.95	0.49
2:H:71:VAL:HG11	2:H:76:PHE:CE2	2.48	0.49
3:L:2:ILE:HD11	3:L:106:GLN:HG3	1.95	0.49
2:H:163:GLU:HB2	2:H:191:TYR:HE2	1.77	0.49
3:L:105:GLN:HB2	3:L:114:PHE:CD1	2.48	0.48
1:A:173:SER:O	1:A:174:THR:CB	2.61	0.48
1:A:247:VAL:O	1:A:282:ARG:HD3	2.12	0.48
2:H:199:VAL:HG21	2:H:209:TYR:CZ	2.49	0.48
1:A:46:SER:HB3	1:A:343:CYS:SG	2.54	0.48
1:A:487:GLN:HB3	1:A:490:ALA:HB2	1.96	0.48
1:A:178:VAL:CG2	3:L:36:ILE:CD1	2.77	0.48
3:L:53:LEU:HA	3:L:71:ILE:HG12	1.96	0.47
2:H:108:ALA:HB2	2:H:116:ASP:OD1	2.14	0.47
1:A:349:VAL:HG12	1:A:350:SER:O	2.14	0.47
3:L:3:VAL:H	3:L:26:SER:CB	2.27	0.47
3:L:36:ILE:HG22	3:L:37:SER:N	2.30	0.47
2:H:109:TYR:HA	2:H:112:TYR:O	2.16	0.46
3:L:217:LEU:HD13	3:L:221:VAL:HG23	1.97	0.46
1:A:48:LEU:HB2	1:A:308:VAL:HB	1.98	0.46
2:H:110:VAL:HG11	2:H:111(B):SER:HB3	1.97	0.46
3:L:164:TRP:O	3:L:170:LEU:HD12	2.15	0.46
1:A:378:GLU:O	1:A:381:LEU:HG	2.15	0.46
1:A:482:VAL:O	1:A:499:ILE:HG12	2.16	0.46
3:L:129:PRO:HB3	3:L:155:PHE:HB3	1.97	0.46
3:L:13:VAL:CG2	3:L:94:LEU:HD12	2.40	0.46
1:A:314:TRP:NE1	1:A:342:TYR:HB2	2.31	0.46
3:L:106:GLN:HG2	3:L:108:ASN:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ILE:HG13	1:A:215:PRO:HD2	1.97	0.46
1:A:328:GLU:H	1:A:328:GLU:CD	2.21	0.46
1:A:83:LEU:HD21	1:A:203:LEU:HD23	1.98	0.45
3:L:11:LEU:O	3:L:120:VAL:HA	2.16	0.45
3:L:124:ARG:HG2	3:L:125:THR:N	2.30	0.45
1:A:174:THR:CG2	3:L:107:TYR:CD1	2.86	0.45
1:A:341:TRP:CZ3	1:A:365:VAL:HG21	2.52	0.45
2:H:161:PHE:O	2:H:215:HIS:HE1	1.99	0.45
3:L:29:VAL:HG13	3:L:106:GLN:HG3	1.98	0.45
3:L:141:LEU:O	3:L:199:LYS:HD2	2.17	0.45
2:H:13:VAL:CG2	2:H:19:LEU:HD22	2.47	0.45
3:L:202:TYR:CE1	3:L:208:TYR:CE1	3.05	0.45
3:L:211:GLU:HG3	3:L:222:THR:OG1	2.17	0.45
3:L:136:PRO:HG3	3:L:146:ALA:HB1	1.98	0.44
2:H:58:TRP:H	2:H:80:ARG:HH11	1.58	0.44
3:L:12:SER:HB3	3:L:121:ASN:OD1	2.17	0.44
1:A:405:SER:HB2	1:A:452:VAL:HG21	2.00	0.44
3:L:191:LEU:HD23	3:L:191:LEU:C	2.43	0.44
1:A:210:GLN:O	1:A:211:SER:O	2.33	0.44
1:A:260:LEU:HD12	1:A:260:LEU:HA	1.79	0.44
3:L:136:PRO:HD3	3:L:148:VAL:HG22	1.99	0.44
1:A:204:LEU:HA	1:A:204:LEU:HD23	1.46	0.44
2:H:95:ARG:HA	2:H:95:ARG:HD3	1.81	0.44
2:H:188:SER:OG	2:H:190:LEU:HB2	2.18	0.44
2:H:72:LYS:C	2:H:75:ARG:H	2.26	0.44
1:A:73:ASP:OD2	1:A:75:LYS:HG3	2.18	0.43
1:A:317:HIS:CE1	1:A:408:THR:HA	2.53	0.43
2:H:54:SER:HB3	2:H:67:TYR:CD2	2.53	0.43
2:H:105:VAL:CG1	2:H:115:LEU:HB3	2.47	0.43
1:A:173:SER:C	1:A:174:THR:HG22	2.43	0.43
1:A:394:LYS:HE3	1:A:394:LYS:HB3	1.55	0.43
2:H:91:MET:HB3	2:H:94:LEU:HD13	2.01	0.43
2:H:110:VAL:HG11	2:H:111(B):SER:CB	2.48	0.43
3:L:6:SER:O	3:L:7:SER:HB3	2.18	0.43
3:L:37:SER:HB3	3:L:83:SER:HB2	2.00	0.43
1:A:216:ASN:OD1	1:A:218:GLU:HB2	2.18	0.43
1:A:523:ALA:HB2	1:A:537:TRP:CE2	2.54	0.43
1:A:47:ALA:O	1:A:366:PHE:HA	2.18	0.43
3:L:25:ALA:O	3:L:85:THR:HG23	2.18	0.43
3:L:27:GLN:HG3	3:L:28:SER:H	1.84	0.43
3:L:197:LEU:HD23	3:L:197:LEU:HA	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:HE2	1:A:294:GLU:HG3	2.01	0.43
1:A:396:MET:HB2	1:A:488:PHE:O	2.19	0.43
1:A:472:GLU:HG2	1:A:473:PRO:HD2	2.01	0.43
3:L:195:LEU:HD12	3:L:195:LEU:HA	1.74	0.43
2:H:186:GLN:HE21	2:H:186:GLN:HB2	1.52	0.43
1:A:211:SER:CA	1:A:212:CYS:HB3	2.49	0.42
2:H:57:THR:O	2:H:57:THR:HG23	2.19	0.42
3:L:171:GLN:HE21	3:L:174:ASN:HD21	1.67	0.42
1:A:479:ASP:HB3	1:A:482:VAL:HG22	2.01	0.42
2:H:161:PHE:HB2	2:H:190:LEU:HD13	2.01	0.42
1:A:175:ASN:O	1:A:176:LYS:C	2.62	0.42
1:A:258:LEU:HD21	1:A:278:VAL:CG2	2.49	0.42
3:L:4:MET:HE2	3:L:4:MET:N	2.35	0.42
2:H:38:THR:HB	2:H:57:THR:CB	2.49	0.42
2:H:96:ALA:O	2:H:99:THR:HG23	2.19	0.42
1:A:37:CYS:HB2	1:A:321:LEU:HD13	2.01	0.42
1:A:88:ASN:O	1:A:92:GLU:HB2	2.19	0.42
1:A:277:ASN:O	1:A:278:VAL:C	2.62	0.42
3:L:214:HIS:CD2	3:L:215:GLN:N	2.85	0.42
1:A:267:THR:HB	1:A:270:GLN:HG3	2.01	0.42
1:A:284:GLN:HB2	1:A:304:PRO:HG3	2.01	0.42
2:H:83:ALA:C	2:H:85:ASN:H	2.28	0.42
2:H:178:VAL:HG22	2:H:197:VAL:HG23	2.00	0.42
3:L:56:GLY:C	3:L:65:SER:H	2.28	0.42
3:L:128:ALA:HB1	3:L:217:LEU:CD2	2.50	0.42
1:A:98:GLN:HG3	1:A:99:SER:N	2.35	0.41
3:L:37:SER:O	3:L:39:LEU:N	2.53	0.41
3:L:94:LEU:HD22	3:L:98:ASP:HB2	2.02	0.41
1:A:83:LEU:HA	1:A:83:LEU:HD13	1.83	0.41
1:A:103:THR:OG1	1:A:105:ASN:ND2	2.53	0.41
1:A:333:CYS:HB3	1:A:398:SER:O	2.20	0.41
1:A:407:ILE:HD11	1:A:457:TYR:HB3	2.02	0.41
2:H:156:LEU:CD2	2:H:158:LYS:HB2	2.49	0.41
2:H:44:GLN:HG3	2:H:49:GLY:O	2.20	0.41
1:A:59:ILE:HD12	1:A:297:LEU:HD23	2.03	0.41
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.89	0.41
1:A:313:CYS:HA	1:A:342:TYR:O	2.21	0.41
1:A:375:LEU:HA	1:A:376:PRO:HD3	1.92	0.41
1:A:394:LYS:HA	1:A:491:SER:HA	2.02	0.41
1:A:442:VAL:CG2	1:A:447:VAL:HG21	2.50	0.41
3:L:52:LEU:O	3:L:71:ILE:HD11	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:PHE:N	1:A:477:PHE:CD2	2.88	0.41
1:A:95:LEU:O	1:A:98:GLN:HG2	2.21	0.40
2:H:170:ASN:HB3	2:H:173:ALA:HB3	2.02	0.40
3:L:94:LEU:HA	3:L:94:LEU:HD23	1.54	0.40
1:A:33:TYR:CE2	1:A:383:ASN:HB3	2.55	0.40
2:H:81:ASP:O	2:H:82:ASN:HB2	2.22	0.40
3:L:95:GLN:HG2	3:L:96:SER:N	2.35	0.40
3:L:166:VAL:HG22	3:L:171:GLN:OE1	2.20	0.40
1:A:475:ILE:HD12	1:A:475:ILE:HA	1.88	0.40
2:H:45:ALA:HB3	2:H:48:LYS:HB2	2.03	0.40
2:H:99:THR:HA	2:H:124:VAL:O	2.22	0.40
3:L:137:SER:HB2	3:L:140:GLN:HB3	2.03	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	486/510 (95%)	462 (95%)	22 (4%)	2 (0%)	30	59
2	H	213/225 (95%)	198 (93%)	14 (7%)	1 (0%)	24	54
3	L	212/214 (99%)	195 (92%)	15 (7%)	2 (1%)	14	41
All	All	911/949 (96%)	855 (94%)	51 (6%)	5 (0%)	24	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	THR
2	H	62	SER
3	L	36	ILE
3	L	38	ASN
1	A	211	SER

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	442/456 (97%)	434 (98%)	8 (2%)	51	69
2	H	182/189 (96%)	180 (99%)	2 (1%)	65	75
3	L	184/186 (99%)	180 (98%)	4 (2%)	45	67
All	All	808/831 (97%)	794 (98%)	14 (2%)	53	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	GLN
1	A	275	SER
1	A	322	CYS
1	A	333	CYS
1	A	350	SER
1	A	362	SER
1	A	425	SER
1	A	541	SER
2	H	38	THR
2	H	186	GLN
3	L	12	SER
3	L	66	THR
3	L	79	SER
3	L	213	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	208	ASN
1	A	240	ASN
1	A	283	GLN
1	A	428	ASN
1	A	437	ASN
1	A	487	GLN

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Mol	Chain	Res	Type
2	H	212	ASN
3	L	48	GLN
3	L	95	GLN
3	L	153	ASN
3	L	168	ASN
3	L	171	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

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	490/510 (96%)	0.18	26 (5%) 32 16	38, 69, 103, 132	0
2	H	217/225 (96%)	0.34	9 (4%) 41 22	47, 68, 100, 117	0
3	L	214/214 (100%)	0.20	9 (4%) 40 21	45, 64, 97, 133	0
All	All	921/949 (97%)	0.22	44 (4%) 35 18	38, 68, 101, 133	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	SER	6.1
2	H	57	THR	5.4
1	A	505	PHE	5.2
1	A	350	SER	5.0
1	A	46	SER	3.9
3	L	79	SER	3.8
1	A	135	GLY	3.7
3	L	230	CYS	3.6
1	A	498	LYS	3.4
2	H	123	LEU	3.3
3	L	36	ILE	3.3
1	A	42	LYS	3.3
1	A	385	ASP	3.1
1	A	70	ASN	3.0
1	A	209	LYS	2.9
1	A	327	LYS	2.8
1	A	326	THR	2.7
2	H	62	SER	2.6
3	L	83	SER	2.6
1	A	445	LYS	2.6
1	A	174	THR	2.6
2	H	122	THR	2.6
2	H	91	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	462	GLN	2.5
1	A	321	LEU	2.5
1	A	429	ARG	2.5
1	A	210	GLN	2.5
3	L	1	GLU	2.4
3	L	92	SER	2.4
1	A	465	LYS	2.4
1	A	463	GLU	2.4
1	A	65	LYS	2.3
1	A	68	LYS	2.3
2	H	16	ARG	2.2
1	A	481	LEU	2.2
1	A	508	LYS	2.2
3	L	29	VAL	2.1
1	A	211	SER	2.1
1	A	175	ASN	2.1
2	H	83	ALA	2.1
2	H	173	ALA	2.1
2	H	95	ARG	2.1
3	L	181	GLU	2.0
3	L	27	GLN	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.