



Full wwPDB EM Validation Report ⓘ

Nov 23, 2025 – 12:16 AM JST

PDB ID : 9U74 / pdb_00009u74
EMDB ID : EMD-63931
Title : Respiratory Syncytial Virus pre-F trimer bound by neutralizing antibody PR306007
Authors : Zheng, Z.; Zixian, S.; Rui, F.; Yu, G.
Deposited on : 2025-03-24
Resolution : 4.08 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

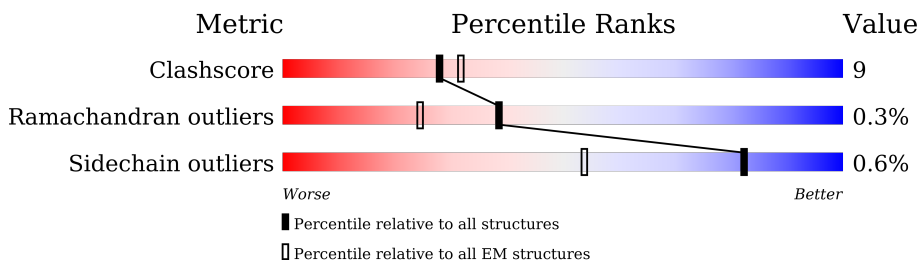
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.08 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	78	
1	C	78	
1	E	78	
2	B	408	
2	D	408	
2	F	408	
3	G	104	
4	H	119	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 F2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	74	Total	C	N	O	S	0	0
			491	312	82	96	1		
1	C	78	Total	C	N	O	S	0	0
			585	368	96	118	3		
1	E	78	Total	C	N	O	S	0	0
			566	356	91	116	3		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	PRO	variant	UNP P03420
C	102	ALA	PRO	variant	UNP P03420
E	102	ALA	PRO	variant	UNP P03420

- Molecule 2 is a protein called Fusion glycoprotein F1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	408	Total	C	N	O	S	0	0
			2771	1762	471	520	18		
2	D	408	Total	C	N	O	S	0	0
			3122	1978	516	608	20		
2	F	408	Total	C	N	O	S	0	0
			3102	1962	513	607	20		

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	155	CYS	SER	conflict	UNP P03420
B	190	PHE	SER	conflict	UNP P03420
B	207	LEU	VAL	conflict	UNP P03420
B	290	CYS	SER	conflict	UNP P03420
B	379	VAL	ILE	conflict	UNP P03420
B	447	VAL	MET	conflict	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
B	514	SER	-	expression tag	UNP P03420
B	515	ALA	-	expression tag	UNP P03420
B	516	ILE	-	expression tag	UNP P03420
B	517	GLY	-	expression tag	UNP P03420
B	518	GLY	-	expression tag	UNP P03420
B	519	TYR	-	expression tag	UNP P03420
B	520	ILE	-	expression tag	UNP P03420
B	521	PRO	-	expression tag	UNP P03420
B	522	GLU	-	expression tag	UNP P03420
B	523	ALA	-	expression tag	UNP P03420
B	524	PRO	-	expression tag	UNP P03420
B	525	ARG	-	expression tag	UNP P03420
B	526	ASP	-	expression tag	UNP P03420
B	527	GLY	-	expression tag	UNP P03420
B	528	GLN	-	expression tag	UNP P03420
B	529	ALA	-	expression tag	UNP P03420
B	530	TYR	-	expression tag	UNP P03420
B	531	VAL	-	expression tag	UNP P03420
B	532	ARG	-	expression tag	UNP P03420
B	533	LYS	-	expression tag	UNP P03420
B	534	ASP	-	expression tag	UNP P03420
B	535	GLY	-	expression tag	UNP P03420
B	536	GLU	-	expression tag	UNP P03420
B	537	TRP	-	expression tag	UNP P03420
B	538	VAL	-	expression tag	UNP P03420
B	539	LEU	-	expression tag	UNP P03420
B	540	LEU	-	expression tag	UNP P03420
B	541	SER	-	expression tag	UNP P03420
B	542	THR	-	expression tag	UNP P03420
B	543	PHE	-	expression tag	UNP P03420
B	544	LEU	-	expression tag	UNP P03420
D	155	CYS	SER	conflict	UNP P03420
D	190	PHE	SER	conflict	UNP P03420
D	207	LEU	VAL	conflict	UNP P03420
D	290	CYS	SER	conflict	UNP P03420
D	379	VAL	ILE	conflict	UNP P03420
D	447	VAL	MET	conflict	UNP P03420
D	514	SER	-	expression tag	UNP P03420
D	515	ALA	-	expression tag	UNP P03420
D	516	ILE	-	expression tag	UNP P03420
D	517	GLY	-	expression tag	UNP P03420
D	518	GLY	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
D	519	TYR	-	expression tag	UNP P03420
D	520	ILE	-	expression tag	UNP P03420
D	521	PRO	-	expression tag	UNP P03420
D	522	GLU	-	expression tag	UNP P03420
D	523	ALA	-	expression tag	UNP P03420
D	524	PRO	-	expression tag	UNP P03420
D	525	ARG	-	expression tag	UNP P03420
D	526	ASP	-	expression tag	UNP P03420
D	527	GLY	-	expression tag	UNP P03420
D	528	GLN	-	expression tag	UNP P03420
D	529	ALA	-	expression tag	UNP P03420
D	530	TYR	-	expression tag	UNP P03420
D	531	VAL	-	expression tag	UNP P03420
D	532	ARG	-	expression tag	UNP P03420
D	533	LYS	-	expression tag	UNP P03420
D	534	ASP	-	expression tag	UNP P03420
D	535	GLY	-	expression tag	UNP P03420
D	536	GLU	-	expression tag	UNP P03420
D	537	TRP	-	expression tag	UNP P03420
D	538	VAL	-	expression tag	UNP P03420
D	539	LEU	-	expression tag	UNP P03420
D	540	LEU	-	expression tag	UNP P03420
D	541	SER	-	expression tag	UNP P03420
D	542	THR	-	expression tag	UNP P03420
D	543	PHE	-	expression tag	UNP P03420
D	544	LEU	-	expression tag	UNP P03420
F	155	CYS	SER	conflict	UNP P03420
F	190	PHE	SER	conflict	UNP P03420
F	207	LEU	VAL	conflict	UNP P03420
F	290	CYS	SER	conflict	UNP P03420
F	379	VAL	ILE	conflict	UNP P03420
F	447	VAL	MET	conflict	UNP P03420
F	514	SER	-	expression tag	UNP P03420
F	515	ALA	-	expression tag	UNP P03420
F	516	ILE	-	expression tag	UNP P03420
F	517	GLY	-	expression tag	UNP P03420
F	518	GLY	-	expression tag	UNP P03420
F	519	TYR	-	expression tag	UNP P03420
F	520	ILE	-	expression tag	UNP P03420
F	521	PRO	-	expression tag	UNP P03420
F	522	GLU	-	expression tag	UNP P03420
F	523	ALA	-	expression tag	UNP P03420

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Chain	Residue	Modelled	Actual	Comment	Reference
F	524	PRO	-	expression tag	UNP P03420
F	525	ARG	-	expression tag	UNP P03420
F	526	ASP	-	expression tag	UNP P03420
F	527	GLY	-	expression tag	UNP P03420
F	528	GLN	-	expression tag	UNP P03420
F	529	ALA	-	expression tag	UNP P03420
F	530	TYR	-	expression tag	UNP P03420
F	531	VAL	-	expression tag	UNP P03420
F	532	ARG	-	expression tag	UNP P03420
F	533	LYS	-	expression tag	UNP P03420
F	534	ASP	-	expression tag	UNP P03420
F	535	GLY	-	expression tag	UNP P03420
F	536	GLU	-	expression tag	UNP P03420
F	537	TRP	-	expression tag	UNP P03420
F	538	VAL	-	expression tag	UNP P03420
F	539	LEU	-	expression tag	UNP P03420
F	540	LEU	-	expression tag	UNP P03420
F	541	SER	-	expression tag	UNP P03420
F	542	THR	-	expression tag	UNP P03420
F	543	PHE	-	expression tag	UNP P03420
F	544	LEU	-	expression tag	UNP P03420

- Molecule 3 is a protein called PR306007 Light chain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	104	Total	C	N	O	S	1	0
			697	436	114	145	2		


- Molecule 4 is a protein called PR306007 Hight chain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	119	Total	C	N	O	S	0	0
			798	496	141	158	3		

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. 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. 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 F2

Chain A: 




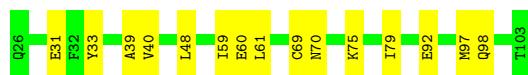
- Molecule 1: Fusion glycoprotein F2

Chain C: 




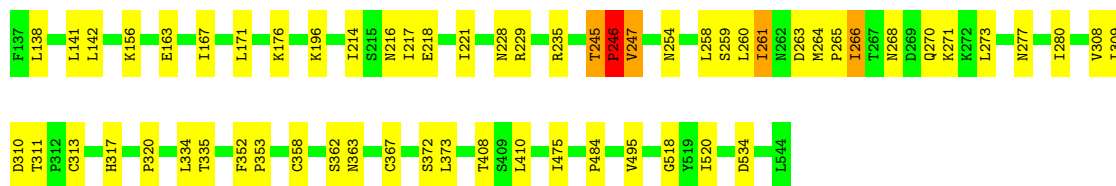
- Molecule 1: Fusion glycoprotein F2

Chain E: 



- Molecule 2: Fusion glycoprotein F1

Chain B: 



- Molecule 2: Fusion glycoprotein F1

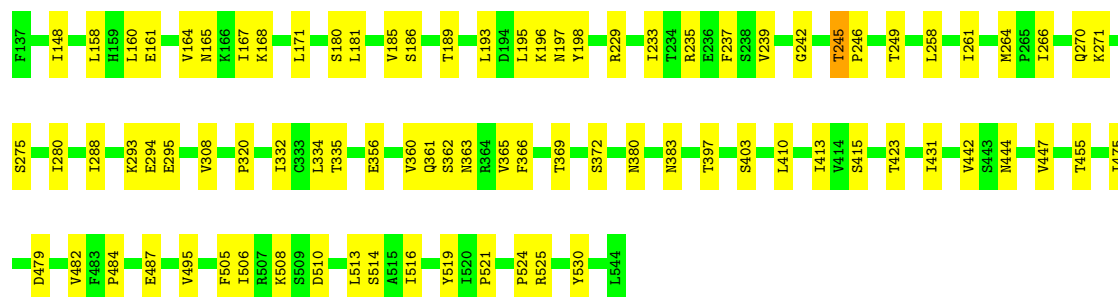
Chain D: 





- Molecule 2: Fusion glycoprotein F1

Chain F: 79% 21%



- Molecule 3: PR306007 Light chain protein

Chain G: 72% 27%



- Molecule 4: PR306007 Hight chain protein

Chain H: 97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

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	0.46	0/497	0.46	0/685
1	C	0.39	0/591	0.55	0/801
1	E	0.55	0/573	0.65	0/782
2	B	0.27	0/2811	0.45	1/3861 (0.0%)
2	D	0.20	0/3172	0.37	0/4308
2	F	0.30	0/3151	0.43	0/4279
3	G	0.57	0/713	0.81	0/982
4	H	0.43	0/817	0.48	1/1124 (0.1%)
All	All	0.33	0/12325	0.47	2/16822 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	246	PRO	N-CA-CB	-5.32	97.66	103.25
4	H	103	SER	N-CA-C	5.23	121.45	113.19

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	491	0	408	9	0
1	C	585	0	567	20	0
1	E	566	0	523	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2771	0	2544	57	0
2	D	3122	0	3130	83	0
2	F	3102	0	3073	58	0
3	G	697	0	601	17	0
4	H	798	0	654	1	0
All	All	12132	0	11500	222	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 (222) 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:B:176:LYS:CE	2:B:263:ASP:OD2	1.64	1.44
2:B:265:PRO:O	2:B:266:ILE:HG23	1.36	1.25
2:B:176:LYS:HE2	2:B:263:ASP:CG	1.69	1.16
2:B:265:PRO:O	2:B:266:ILE:CG2	2.06	1.02
2:B:176:LYS:HE2	2:B:263:ASP:OD2	0.78	0.96
2:B:258:LEU:O	2:B:261:ILE:CG2	2.20	0.89
2:F:380:ASN:O	2:F:383:ASN:HB3	1.74	0.88
2:D:507:ARG:O	2:D:507:ARG:NH1	2.05	0.87
2:B:317:HIS:HD1	2:B:408:THR:HG22	1.41	0.85
3:G:18:ARG:HA	3:G:75:ILE:O	1.78	0.82
2:B:258:LEU:HA	2:B:261:ILE:HG22	1.64	0.80
2:B:258:LEU:O	2:B:261:ILE:HG23	1.80	0.80
2:B:265:PRO:C	2:B:266:ILE:HG23	2.08	0.78
2:B:258:LEU:O	2:B:261:ILE:HG22	1.85	0.76
2:F:165:ASN:HA	2:F:168:LYS:HE2	1.69	0.74
2:B:254:ASN:ND2	1:E:92:GLU:OE1	2.21	0.73
1:C:92:GLU:HA	1:C:95:LEU:HD23	1.71	0.71
2:B:258:LEU:HA	2:B:261:ILE:CG2	2.22	0.69
2:B:334:LEU:HD22	2:B:475:ILE:HD13	1.74	0.69
2:D:176:LYS:NZ	2:D:263:ASP:OD2	2.24	0.69
2:D:164:VAL:HG21	2:D:293:LYS:HD3	1.74	0.67
2:F:362:SER:OG	2:F:363:ASN:N	2.26	0.67
2:B:258:LEU:CA	2:B:261:ILE:HG22	2.24	0.67
2:B:358:CYS:HA	2:B:367:CYS:HB3	1.77	0.67
2:B:258:LEU:C	2:B:261:ILE:HG22	2.19	0.67
2:D:267:THR:OG1	2:D:269:ASP:OD1	2.09	0.67
2:B:176:LYS:HE3	2:B:263:ASP:OD2	1.90	0.66
2:D:521:PRO:HD2	2:D:532:ARG:HH22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:266:ILE:HD12	2:F:270:GLN:HB2	1.77	0.65
3:G:19:VAL:HG12	3:G:75:ILE:HB	1.79	0.65
3:G:22:THR:HG22	3:G:72:THR:HG22	1.78	0.65
2:D:243:VAL:HG22	2:D:288:ILE:HG22	1.79	0.64
2:B:216:ASN:OD1	2:B:217:ILE:N	2.26	0.64
1:C:53:TYR:HB2	2:D:305:LEU:HD11	1.79	0.63
1:A:62:SER:OG	2:B:196:LYS:HA	1.98	0.63
2:D:362:SER:OG	2:D:363:ASN:N	2.31	0.63
2:D:266:ILE:O	2:D:271:LYS:NZ	2.29	0.63
3:G:35:TRP:HB2	3:G:48:ILE:HB	1.81	0.63
2:D:530:TYR:HB3	2:D:537:TRP:HB2	1.80	0.62
2:F:293:LYS:HG3	2:F:294:GLU:OE1	1.99	0.62
2:B:235:ARG:HG2	2:B:235:ARG:HH11	1.64	0.61
3:G:89:GLN:HG2	3:G:90:GLN:H	1.66	0.60
2:B:217:ILE:HG22	2:B:218:GLU:H	1.66	0.60
2:D:246:PRO:HB3	2:D:283:GLN:HA	1.83	0.59
2:F:245:THR:HG23	2:F:246:PRO:HD3	1.85	0.59
2:B:534:ASP:HA	2:D:525:ARG:HA	1.85	0.58
2:F:320:PRO:HA	2:F:335:THR:HG22	1.86	0.58
2:F:484:PRO:HG2	2:F:495:VAL:HG23	1.86	0.58
2:F:360:VAL:HG12	2:F:365:VAL:HG23	1.86	0.57
2:B:484:PRO:HG2	2:B:495:VAL:HG13	1.85	0.57
1:C:78:LEU:HD21	2:D:220:VAL:HG13	1.86	0.57
2:D:180:SER:HA	2:D:186:SER:HA	1.85	0.57
1:E:40:VAL:HG21	2:F:383:ASN:OD1	2.05	0.56
1:A:46:SER:OG	2:B:311:THR:N	2.37	0.56
1:C:72:THR:HA	1:C:76:VAL:HG23	1.86	0.56
1:E:31:GLU:OE1	1:E:33:TYR:OH	2.20	0.56
2:D:518:GLY:HA2	2:F:521:PRO:HA	1.87	0.56
1:C:76:VAL:O	1:C:80:LYS:NZ	2.38	0.56
1:C:71:GLY:O	2:D:212:CYS:SG	2.65	0.55
2:D:200:ASP:OD1	2:D:201:LYS:N	2.39	0.55
2:F:168:LYS:NZ	2:F:294:GLU:OE2	2.39	0.55
2:F:294:GLU:HG2	2:F:295:GLU:OE1	2.06	0.55
2:D:196:LYS:NZ	2:D:200:ASP:OD2	2.36	0.55
1:C:78:LEU:HA	1:C:81:GLN:HB2	1.88	0.54
2:F:410:LEU:O	2:F:444:ASN:ND2	2.40	0.54
2:F:334:LEU:HD22	2:F:475:ILE:HD13	1.89	0.54
2:D:449:THR:HB	2:D:456:LEU:HD11	1.90	0.54
2:D:196:LYS:HA	2:D:199:ILE:HG22	1.88	0.54
2:B:268:ASN:O	2:B:271:LYS:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:ILE:HG23	2:F:193:LEU:HB3	1.90	0.54
1:E:48:LEU:HD11	2:F:308:VAL:HB	1.90	0.54
2:B:260:LEU:O	2:B:264:MET:HG2	2.08	0.54
2:D:521:PRO:HB2	2:D:537:TRP:HZ3	1.73	0.53
2:D:216:ASN:O	2:D:219:THR:OG1	2.26	0.53
2:D:233:ILE:HD13	2:D:251:MET:HG2	1.90	0.53
2:D:484:PRO:HD3	2:D:499:ILE:HD11	1.90	0.53
2:D:171:LEU:HD23	2:D:171:LEU:O	2.09	0.53
2:F:235:ARG:O	2:F:239:VAL:HG23	2.08	0.52
3:G:34:ALA:HB3	3:G:89:GLN:HB3	1.92	0.52
2:D:253:THR:OG1	2:D:256:GLU:OE1	2.18	0.52
2:D:463:GLU:OE1	2:D:464:GLY:N	2.43	0.52
2:D:334:LEU:HD11	2:D:395:ILE:HB	1.91	0.52
2:F:280:ILE:HD11	2:F:361:GLN:HE21	1.73	0.52
2:B:176:LYS:HZ1	2:B:259:SER:HB3	1.76	0.51
2:B:246:PRO:O	2:B:247:VAL:C	2.52	0.51
2:D:356:GLU:N	2:D:356:GLU:OE1	2.43	0.51
2:F:229:ARG:O	2:F:233:ILE:HG12	2.11	0.51
2:B:228:ASN:OD1	2:B:229:ARG:N	2.43	0.51
2:D:338:ASP:OD2	2:D:342:TYR:OH	2.25	0.51
4:H:73:GLN:O	4:H:77:SER:N	2.44	0.51
2:D:323:THR:OG1	2:D:331:ASN:OD1	2.25	0.51
2:B:245:THR:O	2:B:246:PRO:C	2.54	0.51
2:D:315:LYS:HD3	2:D:317:HIS:HE2	1.75	0.50
2:B:245:THR:OG1	2:B:246:PRO:HD2	2.12	0.50
2:D:252:LEU:HD21	2:D:257:LEU:HB2	1.94	0.50
1:C:76:VAL:HG11	2:D:212:CYS:C	2.36	0.50
2:D:257:LEU:O	2:D:261:ILE:HD12	2.12	0.50
2:D:520:ILE:HB	2:D:532:ARG:CZ	2.41	0.50
2:D:261:ILE:HA	2:D:264:MET:HB2	1.94	0.49
2:D:160:LEU:O	2:D:161:GLU:HG3	2.12	0.49
2:D:521:PRO:HD2	2:D:532:ARG:NH2	2.25	0.49
2:F:516:ILE:HD13	2:F:519:TYR:HE2	1.77	0.49
2:B:176:LYS:NZ	2:B:259:SER:HB3	2.27	0.49
1:E:69:CYS:SG	1:E:70:ASN:N	2.85	0.49
2:B:218:GLU:HA	2:B:221:ILE:HB	1.95	0.49
2:B:277:ASN:HB3	2:B:280:ILE:HG22	1.94	0.49
2:D:494:GLN:O	2:D:497:GLU:HG3	2.13	0.49
2:D:273:LEU:HD13	2:D:364:ARG:HH11	1.78	0.49
1:C:75:LYS:HD2	2:D:220:VAL:HG21	1.95	0.48
1:C:28:ILE:HG22	2:D:410:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:507:ARG:HH12	2:D:511:GLU:HB2	1.78	0.48
2:F:510:ASP:O	2:F:514:SER:OG	2.27	0.48
2:B:142:LEU:HD21	2:B:353:PRO:HG2	1.96	0.47
2:D:294:GLU:HG2	2:D:295:GLU:N	2.29	0.47
2:D:387:PHE:HE2	2:D:474:ILE:HD11	1.79	0.47
1:E:97:MET:HG2	1:E:98:GLN:N	2.29	0.47
2:F:180:SER:HA	2:F:186:SER:HA	1.96	0.47
2:D:181:LEU:N	2:D:185:VAL:O	2.45	0.47
2:F:160:LEU:O	2:F:161:GLU:HG3	2.15	0.47
2:F:258:LEU:HD23	2:F:261:ILE:HD11	1.95	0.47
2:B:373:LEU:HD22	2:D:402:VAL:HG11	1.96	0.47
2:F:171:LEU:HD23	2:F:171:LEU:O	2.14	0.47
3:G:2:ILE:HD13	3:G:92:ASN:CB	2.45	0.47
1:C:60:GLU:HG3	2:D:196:LYS:HB3	1.97	0.47
2:D:269:ASP:OD1	2:D:269:ASP:N	2.48	0.47
2:B:171:LEU:HD23	2:B:171:LEU:O	2.15	0.47
2:B:518:GLY:HA2	2:D:521:PRO:HA	1.98	0.46
2:F:356:GLU:OE2	2:F:356:GLU:N	2.38	0.46
2:B:273:LEU:HD22	2:B:309:ILE:HG12	1.98	0.46
2:D:289:MET:HE1	2:D:297:LEU:HD11	1.98	0.46
2:F:369:THR:O	2:F:372:SER:OG	2.31	0.46
3:G:37:GLN:HB3	3:G:47:LEU:HD11	1.98	0.46
2:B:138:LEU:HD12	2:B:141:LEU:HD12	1.98	0.45
2:D:309:ILE:HG13	2:D:310:ASP:CG	2.41	0.45
2:F:332:ILE:HG13	2:F:475:ILE:HD11	1.97	0.45
3:G:17:ASP:H	3:G:78:LEU:H	1.64	0.45
2:F:181:LEU:N	2:F:185:VAL:O	2.47	0.45
2:B:156:LYS:HE2	2:B:156:LYS:HB2	1.82	0.45
2:D:440:ASP:OD1	2:D:441:TYR:N	2.45	0.45
1:E:61:LEU:N	2:F:295:GLU:O	2.41	0.45
2:F:397:THR:OG1	2:F:487:GLU:OE1	2.33	0.45
2:B:320:PRO:HA	2:B:335:THR:HG22	1.99	0.45
2:B:352:PHE:CE1	2:B:372:SER:HB3	2.50	0.45
1:C:89:ALA:O	1:C:93:LEU:HD23	2.16	0.45
2:B:263:ASP:HA	3:G:32:TRP:HE1	1.82	0.45
1:C:49:ARG:HE	2:D:368:ASP:CG	2.24	0.45
2:D:408:THR:O	2:D:460:ASN:ND2	2.50	0.45
2:D:395:ILE:HD11	2:D:495:VAL:HG21	1.99	0.45
2:F:237:PHE:HD1	2:F:242:GLY:HA2	1.81	0.45
2:D:273:LEU:HD13	2:D:364:ARG:NH1	2.33	0.44
2:D:354:GLN:O	2:D:357:THR:HG22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:235:ARG:NH1	2:F:249:THR:OG1	2.50	0.44
1:E:75:LYS:O	1:E:79:ILE:HG12	2.17	0.44
2:B:163:GLU:O	2:B:167:ILE:HG12	2.18	0.44
2:B:235:ARG:HG2	2:B:235:ARG:NH1	2.32	0.44
1:C:46:SER:HB3	2:D:313:CYS:SG	2.58	0.44
2:B:261:ILE:HD11	2:B:271:LYS:HE3	1.99	0.44
2:D:333:CYS:O	2:D:397:THR:OG1	2.31	0.44
2:D:183:ASN:OD1	2:D:185:VAL:HG22	2.18	0.44
2:D:511:GLU:O	2:D:514:SER:OG	2.22	0.44
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.84	0.43
2:F:148:ILE:HB	2:F:288:ILE:HD11	1.99	0.43
2:F:261:ILE:HA	2:F:264:MET:HG2	1.99	0.43
3:G:55:GLN:O	3:G:58:VAL:HG12	2.17	0.43
2:F:164:VAL:HA	2:F:167:ILE:HG22	2.00	0.43
1:A:46:SER:HB3	2:B:313:CYS:SG	2.59	0.43
1:C:76:VAL:HG11	2:D:212:CYS:HA	2.01	0.43
1:A:45:LEU:HD12	2:B:310:ASP:HA	2.00	0.43
1:C:77:LYS:HD2	1:C:77:LYS:HA	1.86	0.43
2:D:534:ASP:HA	2:F:525:ARG:HA	2.01	0.43
1:A:48:LEU:HD12	2:B:308:VAL:HB	2.01	0.43
2:B:520:ILE:HG22	2:D:522:GLU:HA	2.01	0.43
2:F:271:LYS:O	2:F:275:SER:OG	2.28	0.43
3:G:89:GLN:HG2	3:G:90:GLN:N	2.33	0.43
2:B:362:SER:OG	2:B:363:ASN:N	2.37	0.42
2:F:403:SER:HA	2:F:415:SER:O	2.18	0.42
2:D:317:HIS:ND1	2:D:408:THR:HG22	2.33	0.42
1:E:39:ALA:HB2	2:F:413:ILE:HD11	2.00	0.42
2:F:160:LEU:C	2:F:161:GLU:HG3	2.43	0.42
1:C:77:LYS:HA	1:C:80:LYS:HZ2	1.83	0.42
2:F:197:ASN:OD1	2:F:198:TYR:N	2.53	0.42
1:C:89:ALA:HA	1:C:92:GLU:CD	2.43	0.42
2:D:164:VAL:HG11	2:D:293:LYS:HE2	2.01	0.42
2:D:292:ILE:HD13	2:D:297:LEU:HD13	2.01	0.42
2:D:293:LYS:HB3	2:D:294:GLU:OE1	2.20	0.42
1:C:84:ASP:OD1	1:C:85:LYS:N	2.53	0.42
3:G:98:GLY:O	3:G:99:GLN:C	2.63	0.42
3:G:36:TYR:O	3:G:86:TYR:HA	2.20	0.41
2:B:266:ILE:HD12	2:B:270:GLN:HB2	2.03	0.41
2:D:479:ASP:HB3	2:D:482:VAL:HG22	2.02	0.41
1:C:45:LEU:HD11	2:D:310:ASP:HA	2.02	0.41
2:F:380:ASN:O	2:F:383:ASN:CB	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:ASN:CG	2:B:217:ILE:N	2.78	0.41
2:F:506:ILE:HD12	2:F:506:ILE:HA	1.92	0.41
1:A:76:VAL:HG13	2:B:214:ILE:HB	2.02	0.41
2:F:505:PHE:HA	2:F:508:LYS:HE2	2.02	0.41
2:D:203:LEU:O	2:D:206:ILE:HG12	2.20	0.41
2:D:280:ILE:HD13	2:D:280:ILE:HA	1.92	0.41
2:F:442:VAL:HG11	2:F:447:VAL:HG11	2.01	0.41
2:F:510:ASP:HA	2:F:513:LEU:HG	2.02	0.41
2:F:524:PRO:HD2	2:F:530:TYR:CD2	2.55	0.41
3:G:91:PHE:O	3:G:92:ASN:C	2.62	0.41
2:D:160:LEU:C	2:D:161:GLU:HG3	2.45	0.41
2:F:193:LEU:HD12	2:F:193:LEU:HA	1.87	0.41
2:F:167:ILE:HD11	2:F:189:THR:OG1	2.20	0.41
2:F:479:ASP:HB3	2:F:482:VAL:HG12	2.03	0.41
2:D:167:ILE:HD11	2:D:189:THR:HG21	2.03	0.41
3:G:46:LEU:C	3:G:47:LEU:HD12	2.46	0.41
2:D:268:ASN:O	2:D:272:LYS:HG3	2.21	0.40
2:D:369:THR:HB	2:F:455:THR:HG22	2.01	0.40
2:D:230:LEU:HA	2:D:233:ILE:HG22	2.04	0.40
2:F:158:LEU:HD23	2:F:158:LEU:HA	1.95	0.40
3:G:8:PRO:O	3:G:101:THR:OG1	2.38	0.40
2:F:280:ILE:HG21	2:F:366:PHE:CD2	2.56	0.40
1:A:69:CYS:O	1:A:70:ASN:C	2.65	0.40
2:D:194:ASP:OD1	2:D:194:ASP:N	2.53	0.40
2:D:266:ILE:HG13	2:D:267:THR:H	1.85	0.40
1:E:60:GLU:OE2	2:F:195:LEU:N	2.48	0.40
2:F:423:THR:HG23	2:F:431:ILE:HG13	2.03	0.40
1:A:30:GLU:CD	2:B:410:LEU:HB2	2.47	0.40
2:D:425:SER:OG	2:D:426:ASN:N	2.55	0.40
1:E:60:GLU:OE2	2:F:196:LYS:N	2.42	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 PDB entries followed by that with respect to all EM entries.

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	72/78 (92%)	65 (90%)	6 (8%)	1 (1%)	9	41
1	C	76/78 (97%)	63 (83%)	13 (17%)	0	100	100
1	E	76/78 (97%)	67 (88%)	9 (12%)	0	100	100
2	B	406/408 (100%)	377 (93%)	26 (6%)	3 (1%)	19	56
2	D	406/408 (100%)	376 (93%)	30 (7%)	0	100	100
2	F	406/408 (100%)	386 (95%)	20 (5%)	0	100	100
3	G	103/104 (99%)	90 (87%)	12 (12%)	1 (1%)	13	48
4	H	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
All	All	1662/1681 (99%)	1539 (93%)	118 (7%)	5 (0%)	38	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	266	ILE
2	B	246	PRO
2	B	247	VAL
3	G	94	TYR
1	A	64	ILE

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 PDB entries followed by that with respect to all EM entries.

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	39/70 (56%)	39 (100%)	0	100	100
1	C	62/70 (89%)	62 (100%)	0	100	100
1	E	57/70 (81%)	57 (100%)	0	100	100
2	B	266/369 (72%)	263 (99%)	3 (1%)	70	80
2	D	361/369 (98%)	361 (100%)	0	100	100
2	F	353/369 (96%)	352 (100%)	1 (0%)	91	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	66/91 (72%)	64 (97%)	2 (3%)	36	57
4	H	66/96 (69%)	65 (98%)	1 (2%)	60	75
All	All	1270/1504 (84%)	1263 (99%)	7 (1%)	82	88

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

Mol	Chain	Res	Type
2	B	245	THR
2	B	246	PRO
2	B	261	ILE
2	F	245	THR
3	G	90	GLN
3	G	96	THR
4	H	103	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
2	B	437	ASN
1	C	88	ASN
2	D	165	ASN
2	D	227	ASN
2	D	228	ASN
2	D	240	ASN
1	E	34	GLN
2	F	165	ASN
2	F	202	GLN
2	F	361	GLN
2	F	371	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 [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.