



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:16 AM UTC

PDB ID : 5NT2 / pdb_00005nt2
Title : Complex of influenza A NS1 with TRIM25 coiled coil domain
Authors : Koliopoulos, M.G.; Rittinger, K.
Deposited on : 2017-04-27
Resolution : 4.26 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

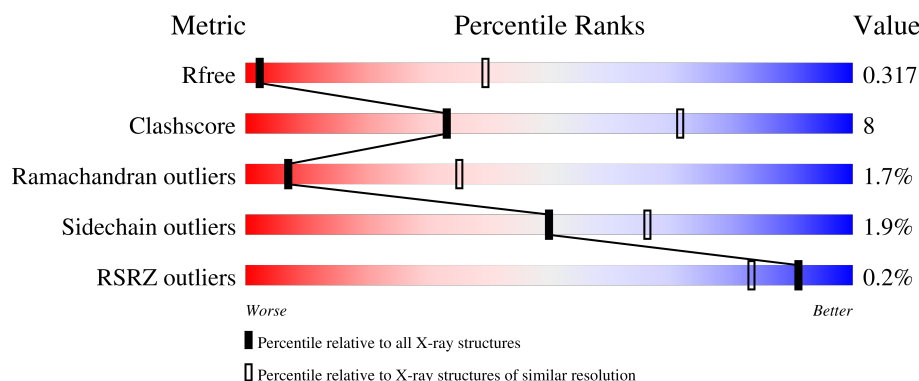
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.26 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	1029 (4.62-3.90)
Clashscore	190562	1074 (4.62-3.90)
Ramachandran outliers	187476	1001 (4.62-3.88)
Sidechain outliers	187428	1021 (4.66-3.86)
RSRZ outliers	180081	1026 (4.62-3.90)

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	C	233	
1	D	233	
1	E	233	
1	F	233	
2	A	193	

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Mol	Chain	Length	Quality of chain
2	I	193	% 67%20%••10%
2	N	193	73%15%•10%
2	V	193	% 72%17%••10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10516 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 Non-structural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	115	Total	C	N	O	S	0	0	0
			894	567	152	169	6			
1	C	115	Total	C	N	O	S	0	0	0
			895	567	152	170	6			
1	D	200	Total	C	N	O	S	0	0	0
			1559	979	274	297	9			
1	E	201	Total	C	N	O	S	0	0	0
			1566	984	275	298	9			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P03496
F	-1	PRO	-	expression tag	UNP P03496
F	0	GLY	-	expression tag	UNP P03496
F	38	ALA	ARG	engineered mutation	UNP P03496
F	41	ALA	LYS	engineered mutation	UNP P03496
F	101	GLU	ASP	variant	UNP P03496
F	187	ALA	TRP	engineered mutation	UNP P03496
C	-2	GLY	-	expression tag	UNP P03496
C	-1	PRO	-	expression tag	UNP P03496
C	0	GLY	-	expression tag	UNP P03496
C	38	ALA	ARG	engineered mutation	UNP P03496
C	41	ALA	LYS	engineered mutation	UNP P03496
C	101	GLU	ASP	variant	UNP P03496
C	187	ALA	TRP	engineered mutation	UNP P03496
D	-2	GLY	-	expression tag	UNP P03496
D	-1	PRO	-	expression tag	UNP P03496
D	0	GLY	-	expression tag	UNP P03496
D	38	ALA	ARG	engineered mutation	UNP P03496
D	41	ALA	LYS	engineered mutation	UNP P03496
D	101	GLU	ASP	variant	UNP P03496
D	187	ALA	TRP	engineered mutation	UNP P03496

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP P03496
E	-1	PRO	-	expression tag	UNP P03496
E	0	GLY	-	expression tag	UNP P03496
E	38	ALA	ARG	engineered mutation	UNP P03496
E	41	ALA	LYS	engineered mutation	UNP P03496
E	101	GLU	ASP	variant	UNP P03496
E	187	ALA	TRP	engineered mutation	UNP P03496

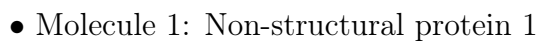
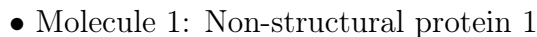
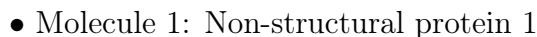
- Molecule 2 is a protein called E3 ubiquitin/ISG15 ligase TRIM25.

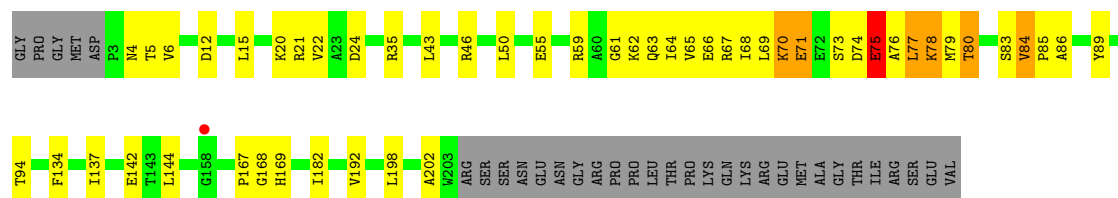
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	173	Total	C	N	O	S	0	0	0
			1399	868	250	277	4			
2	A	173	Total	C	N	O	S	0	0	0
			1401	869	250	278	4			
2	V	173	Total	C	N	O	S	0	0	0
			1401	869	250	278	4			
2	N	173	Total	C	N	O	S	0	0	0
			1401	869	250	278	4			

There are 16 discrepancies between the modelled and reference sequences:

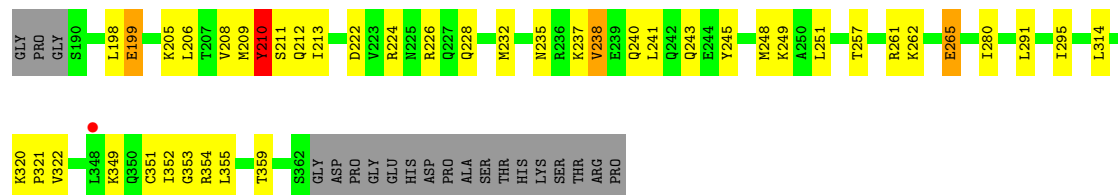
Chain	Residue	Modelled	Actual	Comment	Reference
I	187	GLY	-	expression tag	UNP Q14258
I	188	PRO	-	expression tag	UNP Q14258
I	189	GLY	-	expression tag	UNP Q14258
I	358	LEU	PRO	variant	UNP Q14258
A	187	GLY	-	expression tag	UNP Q14258
A	188	PRO	-	expression tag	UNP Q14258
A	189	GLY	-	expression tag	UNP Q14258
A	358	LEU	PRO	variant	UNP Q14258
V	187	GLY	-	expression tag	UNP Q14258
V	188	PRO	-	expression tag	UNP Q14258
V	189	GLY	-	expression tag	UNP Q14258
V	358	LEU	PRO	variant	UNP Q14258
N	187	GLY	-	expression tag	UNP Q14258
N	188	PRO	-	expression tag	UNP Q14258
N	189	GLY	-	expression tag	UNP Q14258
N	358	LEU	PRO	variant	UNP Q14258

- Molecule 1: Non-structural protein 1

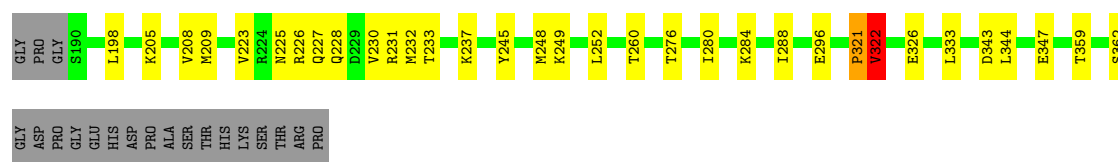




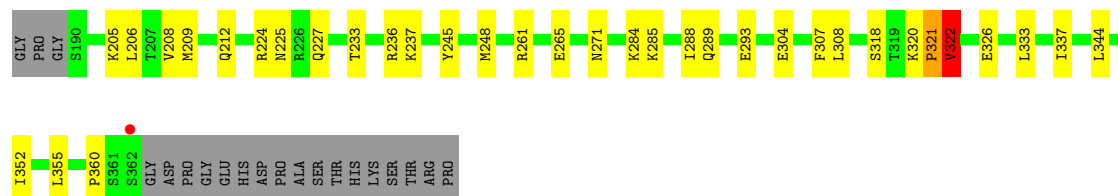
• Molecule 2: E3 ubiquitin/ISG15 ligase TRIM25



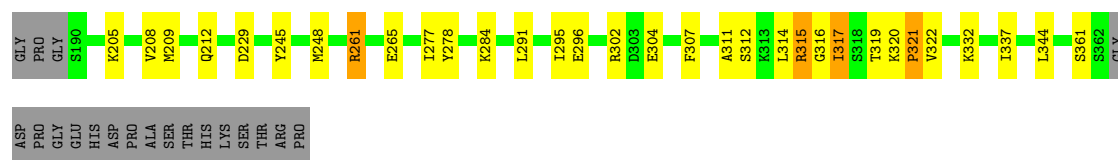
• Molecule 2: E3 ubiquitin/ISG15 ligase TRIM25



• Molecule 2: E3 ubiquitin/ISG15 ligase TRIM25



• Molecule 2: E3 ubiquitin/ISG15 ligase TRIM25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.26Å 76.30Å 92.07Å 100.04° 93.71° 111.14°	Depositor
Resolution (Å)	61.68 – 4.26 61.68 – 4.26	Depositor EDS
% Data completeness (in resolution range)	98.1 (61.68-4.26) 98.0 (61.68-4.26)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.270 , 0.309 0.273 , 0.317	Depositor DCC
R_{free} test set	636 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	122.2	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 111.2	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	0.91	EDS
Total number of atoms	10516	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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	C	0.15	0/907	0.41	0/1226
1	D	0.19	0/1581	0.49	0/2136
1	E	0.19	0/1589	0.52	3/2147 (0.1%)
1	F	0.13	0/906	0.35	0/1224
2	A	0.21	0/1413	0.48	0/1892
2	I	0.23	0/1411	0.59	1/1889 (0.1%)
2	N	0.21	0/1413	0.47	0/1892
2	V	0.20	0/1413	0.46	0/1892
All	All	0.20	0/10633	0.49	4/14298 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	84	VAL	C-N-CD	-6.33	106.68	120.60
2	I	210	TYR	CA-CB-CG	6.12	124.92	113.90
1	E	84	VAL	CA-C-N	6.05	141.53	127.00
1	E	84	VAL	C-N-CA	6.05	141.53	127.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	71	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	E	73	SER	Peptide

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	C	895	0	921	12	0
1	D	1559	0	1586	30	0
1	E	1566	0	1594	36	0
1	F	894	0	921	9	0
2	A	1401	0	1450	28	0
2	I	1399	0	1446	33	0
2	N	1401	0	1450	30	0
2	V	1401	0	1450	28	0
All	All	10516	0	10818	167	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 (167) 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:I:261:ARG:NH2	2:N:361:SER:OG	2.17	0.77
1:D:68:ILE:HA	1:D:70:LYS:H	1.52	0.74
2:I:224:ARG:NH2	2:N:278:TYR:OH	2.23	0.72
2:N:315:ARG:HG3	2:N:316:GLY:H	1.56	0.70
1:D:19:ARG:NH1	1:D:39:ASP:OD2	2.24	0.69
2:I:245:TYR:HA	2:I:248:MET:HE3	1.75	0.68
1:D:71:GLU:HA	1:D:72:GLU:HB3	1.76	0.67
1:D:63:GLN:OE1	1:D:67:ARG:NH2	2.29	0.66
1:E:61:GLY:HA2	1:E:64:ILE:HG22	1.77	0.66
2:I:295:ILE:HG12	2:I:314:LEU:HD13	1.79	0.65
1:F:124:MET:HG2	1:F:188:ASN:HB3	1.76	0.65
2:I:320:LYS:HD3	2:N:212:GLN:HE22	1.61	0.64
1:D:83:SER:OG	1:D:84:VAL:N	2.31	0.64
2:A:245:TYR:HA	2:A:248:MET:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:205:LYS:HE2	2:N:209:MET:HE3	1.81	0.61
1:E:80:THR:HG22	1:E:84:VAL:HA	1.82	0.61
1:E:75:GLU:HG3	1:E:76:ALA:N	2.16	0.61
1:E:198:LEU:O	1:E:202:ALA:HB3	2.00	0.61
2:I:351:CYS:O	2:I:353:GLY:N	2.34	0.60
2:I:212:GLN:HE22	2:N:320:LYS:HD2	1.67	0.60
1:C:95:LEU:HD21	2:N:277:ILE:HG21	1.83	0.60
2:I:262:LYS:HA	2:I:265:GLU:OE2	2.02	0.59
2:I:222:ASP:OD2	2:I:226:ARG:NH1	2.36	0.59
1:D:40:GLN:O	1:D:44:ARG:HG2	2.03	0.59
1:C:147:LEU:HB3	1:C:160:ILE:HB	1.86	0.58
1:D:182:ILE:HG12	1:D:192:VAL:HG11	1.86	0.57
2:A:344:LEU:HD22	2:V:355:LEU:HD22	1.87	0.57
2:A:362:SER:HB3	2:V:265:GLU:OE1	2.04	0.56
2:A:343:ASP:O	2:A:347:GLU:HG2	2.05	0.56
2:A:228:GLN:NE2	2:A:232:MET:HE3	2.21	0.56
2:A:233:THR:O	2:A:237:LYS:HG2	2.05	0.56
1:E:94:THR:HB	2:A:326:GLU:CD	2.31	0.55
1:D:12:ASP:OD2	1:E:35:ARG:NH2	2.38	0.55
2:V:233:THR:O	2:V:237:LYS:HG2	2.07	0.55
2:N:245:TYR:HA	2:N:248:MET:HE3	1.88	0.55
2:N:295:ILE:HG22	2:N:314:LEU:HB3	1.89	0.55
1:D:170:THR:HG22	2:A:260:THR:HG21	1.89	0.54
1:C:182:ILE:HG23	1:C:192:VAL:HG11	1.89	0.54
2:I:209:MET:O	2:I:213:ILE:HG23	2.07	0.54
2:A:359:THR:HG21	2:V:337:ILE:HD11	1.89	0.54
1:C:97:GLU:HA	1:C:100:ARG:HH21	1.72	0.53
2:A:205:LYS:HA	2:A:208:VAL:HG12	1.90	0.53
2:V:245:TYR:HA	2:V:248:MET:HE3	1.89	0.53
1:F:137:ILE:HG22	1:F:142:GLU:HB2	1.90	0.53
1:C:137:ILE:HG22	1:C:142:GLU:HB2	1.91	0.53
1:D:15:LEU:HD22	1:E:15:LEU:HD22	1.91	0.52
1:D:79:MET:HB3	1:E:63:GLN:HB2	1.92	0.51
2:I:235:ASN:HA	2:I:238:VAL:HG13	1.93	0.51
1:D:124:MET:HG2	1:D:188:ASN:HB3	1.93	0.51
1:E:182:ILE:HG12	1:E:192:VAL:HG11	1.93	0.51
2:A:223:VAL:O	2:A:227:GLN:HG2	2.11	0.51
1:D:66:GLU:N	1:D:70:LYS:HE3	2.26	0.51
2:A:198:LEU:HD12	2:V:308:LEU:HD23	1.92	0.50
1:E:77:LEU:O	1:E:79:MET:N	2.44	0.50
2:I:205:LYS:HA	2:I:208:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:224:ARG:HD3	2:V:227:GLN:NE2	2.26	0.49
1:E:6:VAL:HG11	1:E:50:LEU:HD21	1.93	0.49
1:D:16:TRP:CH2	1:D:20:LYS:HD2	2.47	0.49
1:D:68:ILE:HD12	1:D:70:LYS:H	1.78	0.49
2:A:205:LYS:O	2:A:209:MET:HG3	2.13	0.49
2:A:252:LEU:HD23	2:V:352:ILE:HD11	1.94	0.49
1:F:94:THR:HB	2:V:326:GLU:CD	2.38	0.49
1:C:90:LEU:HD21	1:C:197:THR:HG21	1.95	0.49
2:I:359:THR:HG21	2:N:337:ILE:HD11	1.95	0.49
1:D:77:LEU:HD22	1:E:59:ARG:HH11	1.77	0.48
1:E:198:LEU:O	1:E:202:ALA:CB	2.61	0.48
2:I:240:GLN:O	2:I:243:GLN:HG2	2.13	0.48
2:I:248:MET:SD	2:N:344:LEU:HD23	2.54	0.48
2:I:349:LYS:O	2:I:351:CYS:O	2.31	0.48
2:A:231:ARG:HG3	2:V:271:ASN:HD21	1.77	0.48
1:D:61:GLY:HA2	1:D:64:ILE:HG22	1.95	0.48
2:I:198:LEU:HD23	2:N:307:PHE:CE2	2.49	0.48
1:E:80:THR:HA	1:E:83:SER:O	2.13	0.48
1:D:76:ALA:HA	1:D:77:LEU:HB3	1.94	0.48
1:D:68:ILE:HA	1:D:70:LYS:N	2.22	0.48
1:E:137:ILE:HG22	1:E:142:GLU:HB2	1.96	0.47
2:I:248:MET:HA	2:I:251:LEU:HD12	1.96	0.47
2:I:199:GLU:CD	2:N:302:ARG:HB2	2.40	0.47
2:I:351:CYS:SG	2:I:354:ARG:NH2	2.86	0.47
2:N:205:LYS:HA	2:N:208:VAL:HG12	1.97	0.47
1:E:84:VAL:HB	2:V:236:ARG:HD2	1.96	0.46
1:C:141:LEU:HB3	1:C:171:ALA:HB2	1.97	0.46
1:F:172:GLU:OE1	1:F:176:ASN:ND2	2.48	0.46
2:I:291:LEU:HD22	2:N:209:MET:HE1	1.98	0.46
1:E:4:ASN:O	1:E:6:VAL:N	2.48	0.46
2:I:352:ILE:HA	2:I:355:LEU:HB3	1.96	0.46
2:V:261:ARG:O	2:V:265:GLU:HG3	2.15	0.46
2:A:228:GLN:HE21	2:A:232:MET:HE3	1.81	0.46
1:D:28:GLY:O	1:E:5:THR:OG1	2.32	0.46
1:E:76:ALA:HB3	1:E:78:LYS:HD3	1.98	0.46
2:V:205:LYS:HA	2:V:208:VAL:HG12	1.98	0.45
2:N:261:ARG:O	2:N:265:GLU:HG3	2.16	0.45
1:E:70:LYS:HA	1:E:70:LYS:HD2	1.59	0.45
2:V:285:LYS:HE2	2:V:289:GLN:NE2	2.30	0.45
2:V:318:SER:HB2	2:V:320:LYS:HE2	1.97	0.45
1:F:89:TYR:CG	2:A:225:ASN:HB3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:321:PRO:HB2	2:A:322:VAL:H	1.54	0.45
1:D:65:VAL:C	1:D:70:LYS:HG2	2.41	0.45
1:E:20:LYS:O	1:E:21:ARG:C	2.59	0.45
2:V:224:ARG:HD3	2:V:227:GLN:HE21	1.82	0.45
1:E:134:PHE:HB3	1:E:144:LEU:HD12	1.99	0.45
1:D:68:ILE:HA	1:D:68:ILE:HD12	1.75	0.44
2:I:245:TYR:O	2:I:249:LYS:HG3	2.17	0.44
2:A:205:LYS:HG2	2:A:209:MET:HE3	1.97	0.44
1:D:89:TYR:HB3	2:N:229:ASP:HB2	1.97	0.44
2:I:206:LEU:HD21	2:N:296:GLU:HG3	1.99	0.44
2:I:210:TYR:O	2:I:213:ILE:HG12	2.18	0.44
1:E:12:ASP:HB3	1:E:43:LEU:HD21	2.00	0.44
1:E:89:TYR:CG	2:V:225:ASN:HB3	2.53	0.44
2:N:304:GLU:O	2:N:307:PHE:HB3	2.17	0.44
1:C:108:LYS:HG3	1:C:121:GLN:HB2	1.98	0.44
2:I:320:LYS:HD3	2:N:212:GLN:NE2	2.29	0.44
2:N:312:SER:O	2:N:315:ARG:HG2	2.18	0.44
2:N:315:ARG:HG3	2:N:316:GLY:N	2.30	0.44
2:I:212:GLN:NE2	2:N:320:LYS:HD2	2.32	0.44
2:A:284:LYS:O	2:A:288:ILE:HG12	2.18	0.43
2:A:288:ILE:HG21	2:V:212:GLN:HE21	1.83	0.43
2:N:307:PHE:O	2:N:311:ALA:N	2.50	0.43
2:I:351:CYS:O	2:I:352:ILE:HB	2.18	0.43
2:A:296:GLU:HG3	2:V:206:LEU:HD11	2.00	0.43
2:A:276:THR:O	2:A:280:ILE:HD13	2.17	0.43
1:E:144:LEU:HB3	1:E:169:HIS:NE2	2.33	0.43
2:V:321:PRO:HB2	2:V:322:VAL:H	1.57	0.43
2:N:314:LEU:HA	2:N:317:ILE:HD11	2.00	0.43
1:D:20:LYS:HG3	1:D:36:LEU:HD21	2.01	0.43
1:E:65:VAL:O	1:E:67:ARG:N	2.51	0.43
2:A:248:MET:SD	2:V:344:LEU:HD23	2.58	0.43
1:E:71:GLU:HG2	1:E:75:GLU:HB3	2.01	0.43
2:N:284:LYS:HE3	2:N:320:LYS:HA	2.00	0.43
1:C:127:ASN:HB2	1:C:152:GLU:CD	2.44	0.42
1:F:98:MET:HE3	1:F:98:MET:HB3	1.84	0.42
1:E:76:ALA:O	1:E:77:LEU:C	2.62	0.42
2:I:237:LYS:O	2:I:241:LEU:HD13	2.19	0.42
2:V:209:MET:O	2:V:212:GLN:HG2	2.19	0.42
2:I:351:CYS:C	2:I:353:GLY:N	2.76	0.42
1:F:129:ILE:HA	1:F:193:ARG:O	2.19	0.42
1:C:118:ARG:NH2	2:I:211:SER:OG	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:VAL:C	1:E:67:ARG:H	2.28	0.42
2:V:304:GLU:O	2:V:307:PHE:HB3	2.20	0.42
1:D:134:PHE:HB3	1:D:144:LEU:HD12	2.01	0.42
1:E:55:GLU:O	1:E:59:ARG:HG2	2.19	0.42
2:A:359:THR:HG22	2:V:333:LEU:HD11	2.01	0.42
2:V:205:LYS:O	2:V:209:MET:HG3	2.19	0.42
2:A:245:TYR:O	2:A:249:LYS:HG3	2.19	0.42
1:E:167:PRO:HA	1:E:168:GLY:HA2	1.76	0.41
1:E:46:ARG:O	1:E:50:LEU:HB2	2.20	0.41
1:E:63:GLN:HE21	1:E:67:ARG:HD2	1.85	0.41
1:C:109:GLN:HG3	1:C:118:ARG:HG2	2.02	0.41
1:D:167:PRO:HA	1:D:168:GLY:HA2	1.76	0.41
2:A:333:LEU:HD11	2:V:360:PRO:HD2	2.02	0.41
2:N:332:LYS:HA	2:N:332:LYS:HD3	1.81	0.41
1:D:137:ILE:HG22	1:D:142:GLU:HB2	2.02	0.41
2:N:291:LEU:O	2:N:295:ILE:HG12	2.21	0.41
1:F:123:ILE:HG13	1:F:157:VAL:HB	2.03	0.41
1:C:134:PHE:CD2	1:C:141:LEU:HD13	2.55	0.41
1:E:75:GLU:HG3	1:E:77:LEU:N	2.34	0.41
2:I:206:LEU:HD21	2:N:295:ILE:HG13	2.03	0.41
2:N:319:THR:C	2:N:321:PRO:HD3	2.46	0.41
2:I:228:GLN:O	2:I:232:MET:HG2	2.20	0.41
2:V:209:MET:HA	2:V:212:GLN:CD	2.46	0.41
2:V:284:LYS:O	2:V:288:ILE:HG12	2.21	0.41
1:D:20:LYS:O	1:D:21:ARG:C	2.62	0.40
1:E:20:LYS:HG2	1:E:24:ASP:HB2	2.03	0.40
1:F:194:VAL:HG23	1:F:199:GLN:HG2	2.04	0.40
1:D:16:TRP:CZ2	1:D:40:GLN:HB2	2.57	0.40
1:D:77:LEU:HD22	1:E:59:ARG:NH1	2.36	0.40
2:A:226:ARG:O	2:A:230:VAL:HG13	2.21	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	C	113/233 (48%)	112 (99%)	1 (1%)	0	100	100
1	D	198/233 (85%)	174 (88%)	19 (10%)	5 (2%)	4	26
1	E	199/233 (85%)	174 (87%)	18 (9%)	7 (4%)	3	20
1	F	113/233 (48%)	112 (99%)	1 (1%)	0	100	100
2	A	171/193 (89%)	166 (97%)	3 (2%)	2 (1%)	10	43
2	I	171/193 (89%)	165 (96%)	4 (2%)	2 (1%)	10	43
2	N	171/193 (89%)	164 (96%)	3 (2%)	4 (2%)	5	28
2	V	171/193 (89%)	166 (97%)	3 (2%)	2 (1%)	10	43
All	All	1307/1704 (77%)	1233 (94%)	52 (4%)	22 (2%)	7	35

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	78	LYS
1	E	85	PRO
2	I	321	PRO
2	A	321	PRO
2	V	321	PRO
2	N	315	ARG
1	D	68	ILE
1	E	66	GLU
2	I	322	VAL
1	D	74	ASP
1	D	76	ALA
1	E	77	LEU
2	N	322	VAL
1	D	79	MET
1	E	86	ALA
2	V	322	VAL
1	E	75	GLU
2	A	322	VAL
2	N	321	PRO
1	E	22	VAL
2	N	317	ILE
1	D	22	VAL

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	C	100/198 (50%)	97 (97%)	3 (3%)	36	57
1	D	170/198 (86%)	168 (99%)	2 (1%)	63	73
1	E	171/198 (86%)	164 (96%)	7 (4%)	27	49
1	F	100/198 (50%)	100 (100%)	0	100	100
2	A	160/175 (91%)	159 (99%)	1 (1%)	78	80
2	I	159/175 (91%)	153 (96%)	6 (4%)	29	51
2	N	160/175 (91%)	159 (99%)	1 (1%)	78	80
2	V	160/175 (91%)	158 (99%)	2 (1%)	61	71
All	All	1180/1492 (79%)	1158 (98%)	22 (2%)	50	66

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	88	ARG
1	C	91	THR
1	C	100	ARG
1	D	68	ILE
1	D	81	MET
1	E	62	LYS
1	E	68	ILE
1	E	69	LEU
1	E	70	LYS
1	E	74	ASP
1	E	75	GLU
1	E	80	THR
2	I	199	GLU
2	I	210	TYR
2	I	238	VAL
2	I	257	THR
2	I	265	GLU
2	I	280	ILE
2	A	322	VAL

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Mol	Chain	Res	Type
2	V	293	GLU
2	V	322	VAL
2	N	261	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	176	ASN
1	E	25	GLN
1	E	176	ASN
2	I	331	HIS
2	A	204	HIS
2	A	227	GLN
2	A	228	GLN
2	V	204	HIS
2	V	227	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

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	C	115/233 (49%)	-0.18	0 100 100	112, 139, 174, 203	0
1	D	200/233 (85%)	-0.16	0 100 100	115, 169, 241, 260	0
1	E	201/233 (86%)	-0.25	1 (0%) 87 75	113, 154, 208, 240	0
1	F	115/233 (49%)	-0.23	0 100 100	112, 140, 178, 196	0
2	A	173/193 (89%)	-0.19	0 100 100	112, 141, 241, 259	0
2	I	173/193 (89%)	-0.10	1 (0%) 85 73	118, 147, 252, 284	0
2	N	173/193 (89%)	-0.11	0 100 100	109, 147, 327, 404	0
2	V	173/193 (89%)	-0.16	1 (0%) 85 73	111, 148, 260, 285	0
All	All	1323/1704 (77%)	-0.17	3 (0%) 91 83	109, 149, 241, 404	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	362	SER	3.1
2	I	348	LEU	2.5
1	E	158	GLY	2.2

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.