



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:50 PM UTC

PDB ID : 6IW1 / pdb_00006iw1
Title : Crystal structure of YFV-17D sE in postfusion state
Authors : Lu, X.S.; Xiao, H.X.; Li, S.H.; Pang, X.F.
Deposited on : 2018-12-04
Resolution : 3.10 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

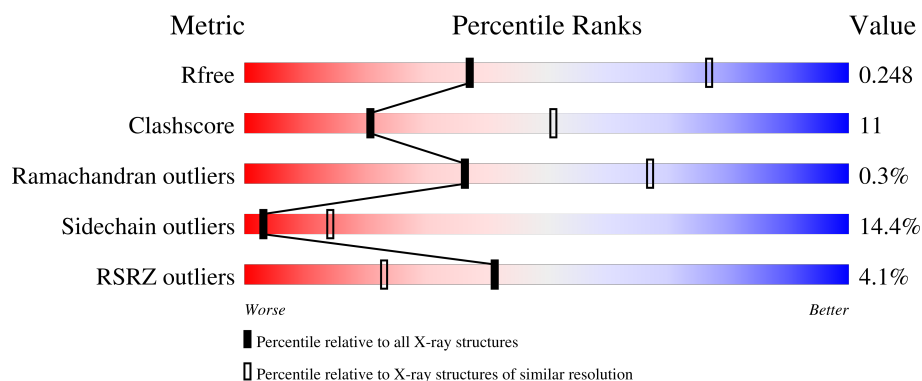
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	395	4% 67% 24% 5% 5%
1	B	395	4% 64% 27% 5% .
1	C	395	4% 62% 28% 5% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8698 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.

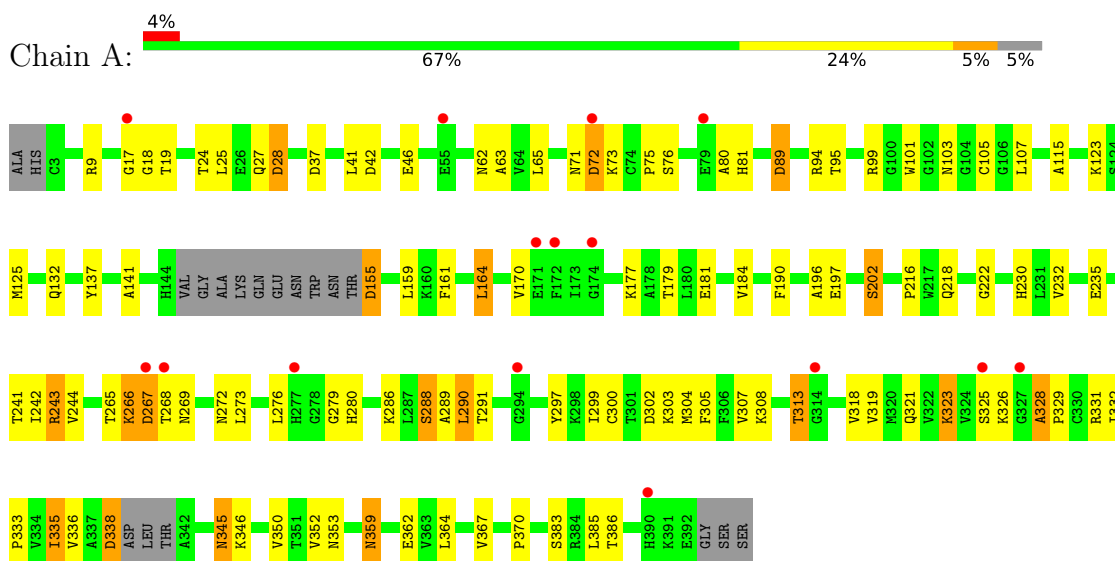
- Molecule 1 is a protein called Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			2895	1818	501	557	19			
1	B	380	Total	C	N	O	S	0	0	0
			2918	1832	504	563	19			
1	C	375	Total	C	N	O	S	0	0	0
			2885	1812	499	555	19			

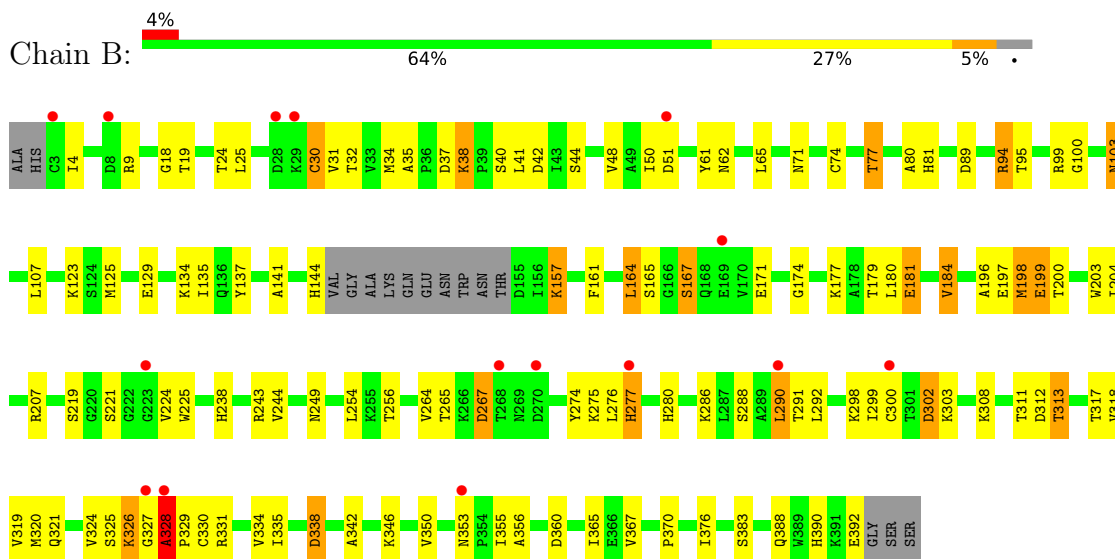
3 Residue-property plots [i](#)

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.

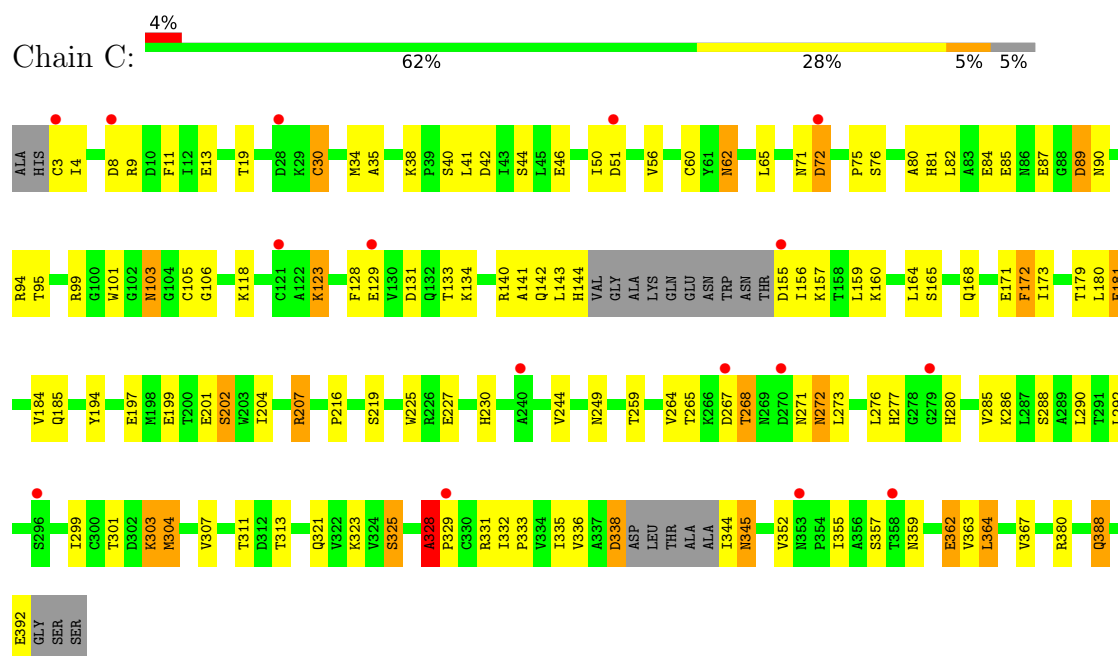
• Molecule 1: Envelope protein E



• Molecule 1: Envelope protein E



• Molecule 1: Envelope protein E



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.56Å 88.28Å 128.95Å 90.00° 107.06° 90.00°	Depositor
Resolution (Å)	39.95 – 3.10 39.95 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.6 (39.95-3.10) 93.1 (39.95-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.215 , 0.254 (Not available) , 0.248	Depositor DCC
R_{free} test set	1328 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8698	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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	0.39	0/2950	0.82	2/3998 (0.1%)
1	B	0.49	1/2974 (0.0%)	0.85	7/4033 (0.2%)
1	C	0.37	0/2940	0.86	3/3984 (0.1%)
All	All	0.42	1/8864 (0.0%)	0.84	12/12015 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	PRO	N-CD	5.17	1.54	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	ALA	CA-C-N	-10.81	107.92	120.13
1	C	328	ALA	C-N-CA	-10.81	107.92	120.13
1	A	266	LYS	N-CA-C	-7.53	102.61	108.78
1	C	272	ASN	N-CA-C	-7.34	102.60	112.94
1	B	221	SER	N-CA-C	-6.74	94.49	107.57
1	B	300	CYS	N-CA-C	-6.26	102.26	110.53
1	B	277	HIS	CB-CA-C	-6.12	98.24	110.42
1	B	328	ALA	CA-C-N	-5.58	112.87	119.84
1	B	328	ALA	C-N-CA	-5.58	112.87	119.84
1	B	277	HIS	N-CA-C	5.47	122.46	110.80
1	B	199	GLU	CB-CA-C	-5.15	110.66	116.63
1	A	279	GLY	N-CA-C	-5.11	105.34	112.18

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	2895	0	2847	68	0
1	B	2918	0	2872	66	0
1	C	2885	0	2839	71	0
All	All	8698	0	8558	192	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 11.

All (192) 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:B:327:GLY:O	1:B:328:ALA:HB2	1.37	1.06
1:A:328:ALA:HB3	1:A:329:PRO:HD2	1.39	1.02
1:B:327:GLY:O	1:B:328:ALA:CB	2.04	1.01
1:A:328:ALA:CB	1:A:329:PRO:CD	2.37	1.01
1:A:328:ALA:CB	1:A:329:PRO:HD2	1.98	0.93
1:A:328:ALA:HB1	1:A:329:PRO:CD	2.00	0.90
1:A:328:ALA:HB1	1:A:329:PRO:HD3	1.60	0.84
1:C:338:ASP:OD1	1:C:338:ASP:N	2.12	0.79
1:B:324:VAL:O	1:B:360:ASP:N	2.18	0.77
1:B:125:MET:HE2	1:B:196:ALA:HB1	1.69	0.75
1:A:328:ALA:HB3	1:A:329:PRO:CD	2.11	0.74
1:A:125:MET:HE2	1:A:196:ALA:HB1	1.69	0.72
1:C:80:ALA:O	1:C:94:ARG:NH2	2.23	0.71
1:A:179:THR:OG1	1:C:9:ARG:NH1	2.23	0.71
1:B:80:ALA:O	1:B:94:ARG:NH2	2.21	0.71
1:A:335:ILE:HG12	1:A:345:ASN:HB3	1.73	0.71
1:B:30:CYS:HB2	1:B:44:SER:HB3	1.72	0.70
1:A:267:ASP:OD2	1:A:273:LEU:HD12	1.92	0.70
1:C:99:ARG:HE	1:C:103:ASN:HD22	1.40	0.70
1:C:99:ARG:HA	1:C:103:ASN:HD21	1.56	0.70
1:C:140:ARG:NH1	1:C:142:GLN:OE1	2.25	0.68
1:A:321:GLN:HG2	1:A:364:LEU:HD23	1.76	0.68
1:C:84:GLU:HB3	1:C:90:ASN:HD22	1.58	0.67
1:A:338:ASP:OD1	1:A:338:ASP:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ASP:O	1:C:271:ASN:ND2	2.29	0.65
1:A:62:ASN:HD22	1:A:63:ALA:N	1.94	0.65
1:C:197:GLU:HG2	1:C:202:SER:HB3	1.78	0.64
1:A:235:GLU:OE2	1:A:243:ARG:NH2	2.31	0.63
1:C:84:GLU:HB3	1:C:90:ASN:ND2	2.14	0.62
1:C:267:ASP:OD1	1:C:268:THR:N	2.30	0.62
1:C:3:CYS:SG	1:C:4:ILE:N	2.73	0.62
1:A:71:ASN:ND2	1:A:81:HIS:O	2.29	0.60
1:A:297:TYR:O	1:B:177:LYS:NZ	2.35	0.60
1:A:353:ASN:O	1:A:353:ASN:ND2	2.35	0.59
1:A:299:ILE:HG23	1:A:333:PRO:HG3	1.83	0.59
1:B:4:ILE:O	1:B:32:THR:N	2.29	0.59
1:B:198:MET:HE1	1:B:254:LEU:HB3	1.84	0.59
1:C:265:THR:OG1	1:C:277:HIS:NE2	2.32	0.58
1:B:224:VAL:HG22	1:B:225:TRP:N	2.18	0.58
1:B:198:MET:HB2	1:B:203:TRP:HZ3	1.67	0.58
1:C:99:ARG:HA	1:C:103:ASN:ND2	2.19	0.57
1:C:325:SER:HA	1:C:359:ASN:HD21	1.68	0.57
1:C:181:GLU:OE1	1:C:286:LYS:NZ	2.37	0.57
1:A:280:HIS:NE2	1:B:164:LEU:O	2.37	0.57
1:A:75:PRO:O	1:A:76:SER:OG	2.20	0.56
1:C:46:GLU:OE2	1:C:140:ARG:HD3	2.05	0.56
1:A:359:ASN:OD1	1:A:359:ASN:N	2.38	0.56
1:C:75:PRO:O	1:C:76:SER:OG	2.22	0.56
1:C:155:ASP:OD2	1:C:155:ASP:N	2.38	0.56
1:B:335:ILE:HD11	1:B:342:ALA:HB1	1.87	0.56
1:A:155:ASP:OD2	1:A:155:ASP:N	2.39	0.55
1:C:51:ASP:OD1	1:C:51:ASP:N	2.39	0.55
1:B:181:GLU:OE1	1:B:286:LYS:NZ	2.39	0.55
1:A:132:GLN:HE21	1:A:190:PHE:HB2	1.70	0.55
1:B:313:THR:OG1	1:B:317:THR:O	2.25	0.54
1:C:336:VAL:H	1:C:345:ASN:HB2	1.73	0.54
1:B:197:GLU:OE2	1:B:274:TYR:OH	2.23	0.54
1:C:101:TRP:NE1	1:C:106:GLY:O	2.35	0.53
1:B:51:ASP:OD1	1:B:51:ASP:N	2.36	0.53
1:C:142:GLN:HB2	1:C:156:ILE:HG22	1.89	0.53
1:A:42:ASP:O	1:A:141:ALA:HA	2.08	0.53
1:C:335:ILE:HG23	1:C:345:ASN:HB3	1.91	0.53
1:A:164:LEU:O	1:C:280:HIS:NE2	2.42	0.52
1:B:65:LEU:HD13	1:B:244:VAL:HG12	1.92	0.52
1:C:42:ASP:O	1:C:141:ALA:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:THR:CG2	1:B:290:LEU:H	2.23	0.52
1:C:321:GLN:HG2	1:C:364:LEU:HD12	1.90	0.52
1:B:9:ARG:HH22	1:B:331:ARG:NH2	2.06	0.52
1:B:40:SER:HB2	1:B:144:HIS:ND1	2.25	0.52
1:B:302:ASP:OD1	1:B:302:ASP:N	2.42	0.52
1:B:390:HIS:NE2	1:B:392:GLU:OE2	2.26	0.52
1:A:267:ASP:C	1:A:269:ASN:H	2.18	0.52
1:C:128:PHE:HE1	1:C:197:GLU:HB2	1.75	0.52
1:C:62:ASN:OD1	1:C:249:ASN:ND2	2.43	0.51
1:A:18:GLY:HA3	1:C:9:ARG:HA	1.92	0.51
1:C:89:ASP:N	1:C:89:ASP:OD1	2.43	0.51
1:A:218:GLN:CG	1:A:222:GLY:O	2.59	0.51
1:A:65:LEU:HD13	1:A:244:VAL:HG12	1.92	0.51
1:A:17:GLY:O	1:A:289:ALA:HB2	2.11	0.51
1:B:320:MET:HE1	1:B:376:ILE:HG21	1.93	0.51
1:A:24:THR:OG1	1:A:352:VAL:HG21	2.11	0.51
1:C:50:ILE:HD11	1:C:276:LEU:HD21	1.92	0.51
1:A:304:MET:O	1:A:385:LEU:HD21	2.12	0.50
1:A:80:ALA:O	1:A:94:ARG:NH2	2.43	0.50
1:B:298:LYS:O	1:B:330:CYS:HB2	2.12	0.50
1:A:302:ASP:HB3	1:A:303:LYS:HG2	1.93	0.50
1:C:19:THR:CG2	1:C:290:LEU:H	2.25	0.50
1:C:194:TYR:CE2	1:C:207:ARG:HG3	2.47	0.50
1:A:89:ASP:N	1:A:89:ASP:OD1	2.44	0.50
1:B:50:ILE:HD11	1:B:276:LEU:HD21	1.95	0.49
1:C:303:LYS:HB3	1:C:325:SER:OG	2.12	0.49
1:B:308:LYS:HB2	1:B:321:GLN:HE21	1.76	0.49
1:C:216:PRO:HD3	1:C:230:HIS:HB2	1.94	0.49
1:C:65:LEU:HA	1:C:118:LYS:O	2.12	0.49
1:C:84:GLU:O	1:C:87:GLU:HG2	2.13	0.49
1:A:350:VAL:HA	1:B:165:SER:HB2	1.95	0.49
1:B:9:ARG:HH22	1:B:331:ARG:HH22	1.60	0.49
1:A:9:ARG:NH1	1:B:179:THR:OG1	2.46	0.49
1:A:72:ASP:OD2	1:A:99:ARG:NH1	2.45	0.49
1:A:159:LEU:HD21	1:A:170:VAL:HG22	1.94	0.49
1:B:74:CYS:O	1:B:77:THR:OG1	2.29	0.49
1:A:336:VAL:H	1:A:345:ASN:HB2	1.76	0.49
1:A:346:LYS:HB2	1:A:370:PRO:HG2	1.95	0.49
1:B:62:ASN:HB3	1:B:123:LYS:HB2	1.94	0.49
1:B:338:ASP:OD1	1:B:338:ASP:N	2.35	0.48
1:C:332:ILE:HD12	1:C:363:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LYS:NZ	1:B:171:GLU:O	2.43	0.48
1:A:9:ARG:HA	1:B:18:GLY:HA3	1.95	0.48
1:C:72:ASP:OD1	1:C:99:ARG:NH1	2.47	0.48
1:A:326:LYS:O	1:A:359:ASN:ND2	2.46	0.48
1:C:304:MET:HE3	1:C:304:MET:HB3	1.72	0.48
1:C:11:PHE:CD2	1:C:292:LEU:HD12	2.48	0.48
1:A:288:SER:O	1:A:290:LEU:HD23	2.13	0.48
1:B:9:ARG:NH1	1:C:179:THR:OG1	2.46	0.48
1:A:350:VAL:HG13	1:B:164:LEU:HD12	1.95	0.47
1:C:131:ASP:HB3	1:C:134:LYS:HB2	1.96	0.47
1:A:62:ASN:HD22	1:A:62:ASN:C	2.22	0.47
1:B:137:TYR:CZ	1:B:161:PHE:HB3	2.49	0.47
1:C:65:LEU:HD13	1:C:244:VAL:HG12	1.97	0.47
1:B:48:VAL:HG12	1:B:276:LEU:HD12	1.96	0.47
1:A:267:ASP:OD2	1:A:273:LEU:HB2	2.14	0.46
1:C:30:CYS:HB2	1:C:44:SER:HB3	1.97	0.46
1:B:19:THR:HG21	1:B:290:LEU:O	2.16	0.46
1:C:19:THR:HG21	1:C:290:LEU:H	1.80	0.46
1:A:286:LYS:HB3	1:C:9:ARG:HB2	1.98	0.46
1:A:303:LYS:HG3	1:A:326:LYS:HE3	1.97	0.46
1:B:326:LYS:HB2	1:B:326:LYS:HE2	1.80	0.46
1:C:123:LYS:NZ	1:C:199:GLU:OE1	2.43	0.46
1:B:38:LYS:HD3	1:B:174:GLY:O	2.17	0.45
1:C:103:ASN:OD1	1:C:103:ASN:N	2.49	0.45
1:A:19:THR:HG23	1:A:289:ALA:HA	1.97	0.45
1:C:328:ALA:HB1	1:C:329:PRO:CD	2.46	0.45
1:A:137:TYR:CZ	1:A:161:PHE:HB3	2.51	0.45
1:B:71:ASN:ND2	1:B:81:HIS:O	2.39	0.45
1:B:267:ASP:HB2	1:B:275:LYS:HZ2	1.80	0.45
1:C:143:LEU:HD11	1:C:172:PHE:HB2	1.99	0.45
1:A:65:LEU:HD11	1:A:232:VAL:HG13	1.99	0.45
1:A:331:ARG:CZ	1:A:353:ASN:HA	2.47	0.44
1:C:204:ILE:HG13	1:C:264:VAL:CG2	2.47	0.44
1:B:61:TYR:HB3	1:B:254:LEU:HD12	2.00	0.44
1:B:224:VAL:CG2	1:B:225:TRP:N	2.81	0.44
1:C:35:ALA:HB3	1:C:38:LYS:HB2	2.00	0.44
1:B:355:ILE:HG22	1:B:356:ALA:N	2.32	0.44
1:B:30:CYS:SG	1:B:31:VAL:N	2.91	0.44
1:A:19:THR:HG21	1:A:290:LEU:O	2.18	0.44
1:A:313:THR:HG23	1:A:319:VAL:HG23	1.99	0.44
1:A:323:LYS:HG3	1:A:362:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:SER:OG	1:B:181:GLU:HG3	2.17	0.44
1:A:307:VAL:HG11	1:A:362:GLU:OE2	2.18	0.43
1:B:267:ASP:HB2	1:B:275:LYS:NZ	2.33	0.43
1:B:62:ASN:HD22	1:B:249:ASN:HA	1.84	0.43
1:C:307:VAL:HG11	1:C:362:GLU:OE2	2.18	0.43
1:B:346:LYS:O	1:B:370:PRO:HG3	2.18	0.43
1:A:101:TRP:HD1	1:A:105:CYS:O	2.02	0.43
1:A:267:ASP:C	1:A:269:ASN:N	2.77	0.43
1:C:299:ILE:HG23	1:C:333:PRO:HG3	2.00	0.43
1:C:180:LEU:HD23	1:C:285:VAL:HG22	2.00	0.43
1:A:28:ASP:OD2	1:A:28:ASP:N	2.51	0.42
1:A:197:GLU:HG2	1:A:202:SER:HB3	2.01	0.42
1:B:19:THR:HG21	1:B:290:LEU:H	1.82	0.42
1:B:137:TYR:CE1	1:B:184:VAL:HG22	2.54	0.42
1:A:159:LEU:HD11	1:A:170:VAL:HG21	2.00	0.42
1:C:99:ARG:NE	1:C:103:ASN:HD22	2.12	0.42
1:B:350:VAL:HA	1:C:165:SER:HB2	2.01	0.42
1:B:35:ALA:HB2	1:B:292:LEU:HD23	2.01	0.42
1:A:267:ASP:OD2	1:A:273:LEU:CD1	2.66	0.42
1:B:204:ILE:HG13	1:B:264:VAL:CG2	2.50	0.42
1:B:42:ASP:O	1:B:141:ALA:HA	2.20	0.41
1:B:313:THR:HG23	1:B:319:VAL:HG23	2.01	0.41
1:B:167:SER:HA	1:B:180:LEU:O	2.20	0.41
1:C:40:SER:HB2	1:C:144:HIS:CD2	2.55	0.41
1:C:50:ILE:O	1:C:273:LEU:HA	2.19	0.41
1:C:60:CYS:HB2	1:C:225:TRP:CZ3	2.55	0.41
1:B:334:VAL:HG21	1:B:365:ILE:HD13	2.01	0.41
1:C:101:TRP:HD1	1:C:105:CYS:O	2.03	0.41
1:A:332:ILE:HA	1:A:333:PRO:HD3	1.92	0.41
1:A:115:ALA:HB2	1:A:242:ILE:HD12	2.02	0.41
1:C:157:LYS:HE2	1:C:171:GLU:O	2.21	0.41
1:B:4:ILE:O	1:B:32:THR:HG22	2.21	0.41
1:B:25:LEU:O	1:B:280:HIS:HB2	2.21	0.41
1:B:100:GLY:N	1:B:103:ASN:OD1	2.42	0.41
1:B:134:LYS:HE2	1:B:134:LYS:HB3	1.82	0.41
1:C:165:SER:OG	1:C:168:GLN:OE1	2.39	0.41
1:C:388:GLN:HE21	1:C:388:GLN:HA	1.86	0.41
1:A:177:LYS:HZ3	1:C:331:ARG:HD2	1.86	0.41
1:C:71:ASN:HD22	1:C:81:HIS:H	1.68	0.41
1:C:82:LEU:O	1:C:85:GLU:HB2	2.20	0.41
1:B:99:ARG:HA	1:B:99:ARG:HD2	1.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LEU:HD23	1:A:107:LEU:H	1.86	0.40
1:C:13:GLU:HG3	1:C:19:THR:HG22	2.02	0.40
1:C:131:ASP:OD1	1:C:133:THR:OG1	2.32	0.40
1:A:216:PRO:HD3	1:A:230:HIS:HB2	2.03	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	371/395 (94%)	361 (97%)	9 (2%)	1 (0%)	36	67
1	B	376/395 (95%)	364 (97%)	11 (3%)	1 (0%)	36	67
1	C	369/395 (93%)	360 (98%)	8 (2%)	1 (0%)	36	67
All	All	1116/1185 (94%)	1085 (97%)	28 (2%)	3 (0%)	36	67

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ALA
1	B	328	ALA
1	C	328	ALA

5.3.2 Protein sidechains [i](#)

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	317/331 (96%)	275 (87%)	42 (13%)	4	17
1	B	320/331 (97%)	273 (85%)	47 (15%)	3	14
1	C	317/331 (96%)	269 (85%)	48 (15%)	3	13
All	All	954/993 (96%)	817 (86%)	137 (14%)	3	14

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	27	GLN
1	A	28	ASP
1	A	37	ASP
1	A	41	LEU
1	A	46	GLU
1	A	72	ASP
1	A	73	LYS
1	A	89	ASP
1	A	95	THR
1	A	103	ASN
1	A	123	LYS
1	A	155	ASP
1	A	164	LEU
1	A	181	GLU
1	A	184	VAL
1	A	202	SER
1	A	241	THR
1	A	243	ARG
1	A	265	THR
1	A	266	LYS
1	A	267	ASP
1	A	268	THR
1	A	272	ASN
1	A	276	LEU
1	A	288	SER
1	A	290	LEU
1	A	291	THR
1	A	300	CYS
1	A	305	PHE
1	A	308	LYS
1	A	313	THR
1	A	318	VAL
1	A	323	LYS

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Mol	Chain	Res	Type
1	A	325	SER
1	A	335	ILE
1	A	338	ASP
1	A	345	ASN
1	A	359	ASN
1	A	367	VAL
1	A	383	SER
1	A	386	THR
1	B	24	THR
1	B	30	CYS
1	B	34	MET
1	B	37	ASP
1	B	38	LYS
1	B	41	LEU
1	B	77	THR
1	B	89	ASP
1	B	94	ARG
1	B	95	THR
1	B	103	ASN
1	B	107	LEU
1	B	129	GLU
1	B	135	ILE
1	B	157	LYS
1	B	164	LEU
1	B	167	SER
1	B	181	GLU
1	B	184	VAL
1	B	198	MET
1	B	199	GLU
1	B	200	THR
1	B	207	ARG
1	B	219	SER
1	B	238	HIS
1	B	243	ARG
1	B	256	THR
1	B	265	THR
1	B	267	ASP
1	B	277	HIS
1	B	288	SER
1	B	290	LEU
1	B	291	THR
1	B	299	ILE

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Mol	Chain	Res	Type
1	B	302	ASP
1	B	303	LYS
1	B	311	THR
1	B	312	ASP
1	B	313	THR
1	B	318	VAL
1	B	325	SER
1	B	326	LYS
1	B	338	ASP
1	B	353	ASN
1	B	367	VAL
1	B	383	SER
1	B	388	GLN
1	C	8	ASP
1	C	30	CYS
1	C	34	MET
1	C	41	LEU
1	C	56	VAL
1	C	62	ASN
1	C	72	ASP
1	C	89	ASP
1	C	95	THR
1	C	103	ASN
1	C	123	LYS
1	C	129	GLU
1	C	159	LEU
1	C	160	LYS
1	C	164	LEU
1	C	172	PHE
1	C	173	ILE
1	C	181	GLU
1	C	184	VAL
1	C	185	GLN
1	C	201	GLU
1	C	202	SER
1	C	207	ARG
1	C	219	SER
1	C	227	GLU
1	C	259	THR
1	C	268	THR
1	C	272	ASN
1	C	288	SER

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Mol	Chain	Res	Type
1	C	301	THR
1	C	303	LYS
1	C	304	MET
1	C	311	THR
1	C	313	THR
1	C	323	LYS
1	C	325	SER
1	C	338	ASP
1	C	344	ILE
1	C	345	ASN
1	C	352	VAL
1	C	355	ILE
1	C	357	SER
1	C	362	GLU
1	C	364	LEU
1	C	367	VAL
1	C	380	ARG
1	C	388	GLN
1	C	392	GLU

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

Mol	Chain	Res	Type
1	A	183	GLN
1	A	230	HIS
1	A	271	ASN
1	B	359	ASN
1	C	71	ASN
1	C	103	ASN
1	C	345	ASN
1	C	359	ASN
1	C	388	GLN

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.

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	377/395 (95%)	0.26	15 (3%)	42 23	22, 56, 106, 163	0
1	B	380/395 (96%)	0.21	15 (3%)	43 24	21, 56, 101, 156	0
1	C	375/395 (94%)	0.35	16 (4%)	40 22	17, 62, 118, 155	0
All	All	1132/1185 (95%)	0.27	46 (4%)	41 23	17, 58, 112, 163	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	51	ASP	5.1
1	C	72	ASP	5.0
1	B	51	ASP	3.8
1	B	277	HIS	3.7
1	C	270	ASP	3.7
1	A	267	ASP	3.4
1	B	270	ASP	3.0
1	A	171	GLU	2.9
1	B	8	ASP	2.9
1	A	327	GLY	2.9
1	C	279	GLY	2.9
1	A	55	GLU	2.8
1	C	329	PRO	2.8
1	A	314	GLY	2.7
1	C	358	THR	2.6
1	B	300	CYS	2.6
1	B	328	ALA	2.6
1	C	353	ASN	2.6
1	A	17	GLY	2.5
1	C	28	ASP	2.5
1	C	3	CYS	2.5
1	B	169	GLU	2.4
1	A	268	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	390	HIS	2.4
1	B	268	THR	2.4
1	B	28	ASP	2.4
1	A	294	GLY	2.4
1	B	29	LYS	2.4
1	A	72	ASP	2.3
1	C	155	ASP	2.3
1	C	267	ASP	2.3
1	A	174	GLY	2.2
1	A	79	GLU	2.2
1	B	223	GLY	2.2
1	A	325	SER	2.2
1	C	129	GLU	2.2
1	B	353	ASN	2.2
1	C	240	ALA	2.2
1	B	3	CYS	2.2
1	C	121	CYS	2.2
1	A	172	PHE	2.2
1	C	296	SER	2.1
1	C	8	ASP	2.1
1	A	277	HIS	2.1
1	B	290	LEU	2.1
1	B	327	GLY	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.