



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:03 PM UTC

PDB ID : 6LGW / pdb_00006lgw
Title : Structure of Rabies virus glycoprotein in complex with neutralizing antibody 523-11 at acidic pH
Authors : Yang, F.L.; Lin, S.; Ye, F.; Yang, J.; Qi, J.X.; Chen, Z.J.; Lin, X.; Wang, J.C.; Yue, D.; Cheng, Y.W.; Chen, Z.M.; Chen, H.; You, Y.; Zhang, Z.L.; Yang, Y.; Yang, M.; Sun, H.L.; Li, Y.H.; Cao, Y.; Yang, S.Y.; Wei, Y.Q.; Gao, G.F.; Lu, G.W.
Deposited on : 2019-12-06
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

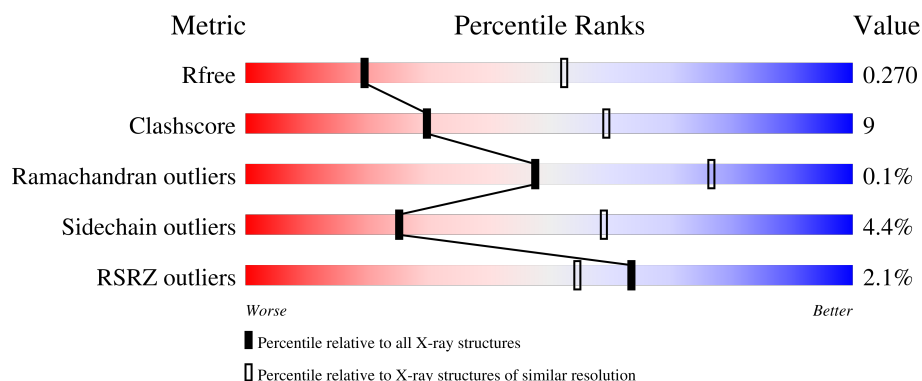
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	A	228	
1	C	228	
2	E	409	
2	F	409	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 9342 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 scFv 523-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1720	1085	286	342	7			
1	C	223	Total	C	N	O	S	0	0	0
			1727	1088	288	344	7			

- Molecule 2 is a protein called Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	368	Total	C	N	O	S	0	0	0
			2902	1837	499	543	23			
2	F	378	Total	C	N	O	S	0	0	0
			2993	1893	520	556	24			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	ALA	-	expression tag	UNP Q5JZZ2
E	-2	ASP	-	expression tag	UNP Q5JZZ2
E	-1	GLU	-	expression tag	UNP Q5JZZ2
E	0	PHE	-	expression tag	UNP Q5JZZ2
E	75	GLY	-	linker	UNP Q5JZZ2
E	76	GLY	-	linker	UNP Q5JZZ2
E	77	SER	-	linker	UNP Q5JZZ2
E	78	GLY	-	linker	UNP Q5JZZ2
E	79	GLY	-	linker	UNP Q5JZZ2
E	121	GLY	-	linker	UNP Q2Z2I1
E	122	GLY	-	linker	UNP Q2Z2I1
E	123	SER	-	linker	UNP Q2Z2I1
E	124	GLY	-	linker	UNP Q2Z2I1
E	125	GLY	-	linker	UNP Q2Z2I1
E	406	HIS	-	expression tag	UNP D8VEC1
E	407	HIS	-	expression tag	UNP D8VEC1

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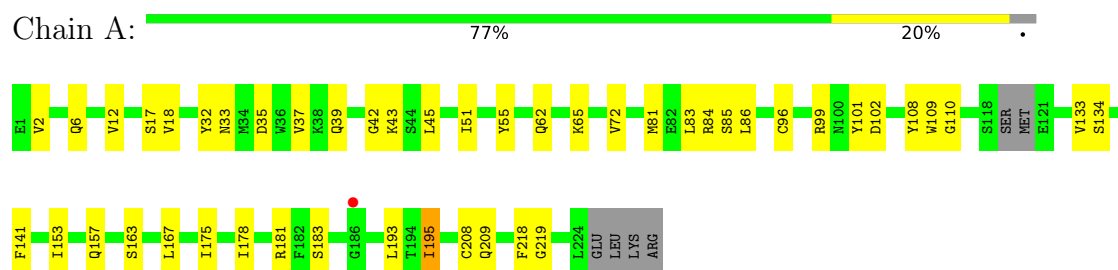
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Chain	Residue	Modelled	Actual	Comment	Reference
E	408	HIS	-	expression tag	UNP D8VEC1
E	409	HIS	-	expression tag	UNP D8VEC1
E	410	HIS	-	expression tag	UNP D8VEC1
E	411	HIS	-	expression tag	UNP D8VEC1
F	-3	ALA	-	expression tag	UNP Q5JZZ2
F	-2	ASP	-	expression tag	UNP Q5JZZ2
F	-1	GLU	-	expression tag	UNP Q5JZZ2
F	0	PHE	-	expression tag	UNP Q5JZZ2
F	75	GLY	-	linker	UNP Q5JZZ2
F	76	GLY	-	linker	UNP Q5JZZ2
F	77	SER	-	linker	UNP Q5JZZ2
F	78	GLY	-	linker	UNP Q5JZZ2
F	79	GLY	-	linker	UNP Q5JZZ2
F	121	GLY	-	linker	UNP Q2Z2I1
F	122	GLY	-	linker	UNP Q2Z2I1
F	123	SER	-	linker	UNP Q2Z2I1
F	124	GLY	-	linker	UNP Q2Z2I1
F	125	GLY	-	linker	UNP Q2Z2I1
F	406	HIS	-	expression tag	UNP D8VEC1
F	407	HIS	-	expression tag	UNP D8VEC1
F	408	HIS	-	expression tag	UNP D8VEC1
F	409	HIS	-	expression tag	UNP D8VEC1
F	410	HIS	-	expression tag	UNP D8VEC1
F	411	HIS	-	expression tag	UNP D8VEC1

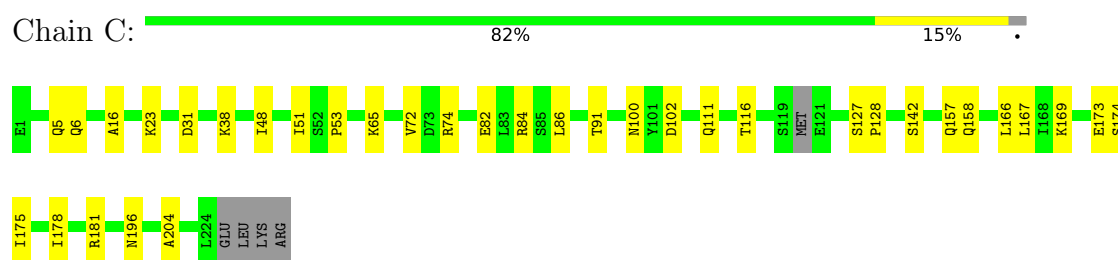
3 Residue-property plots

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.

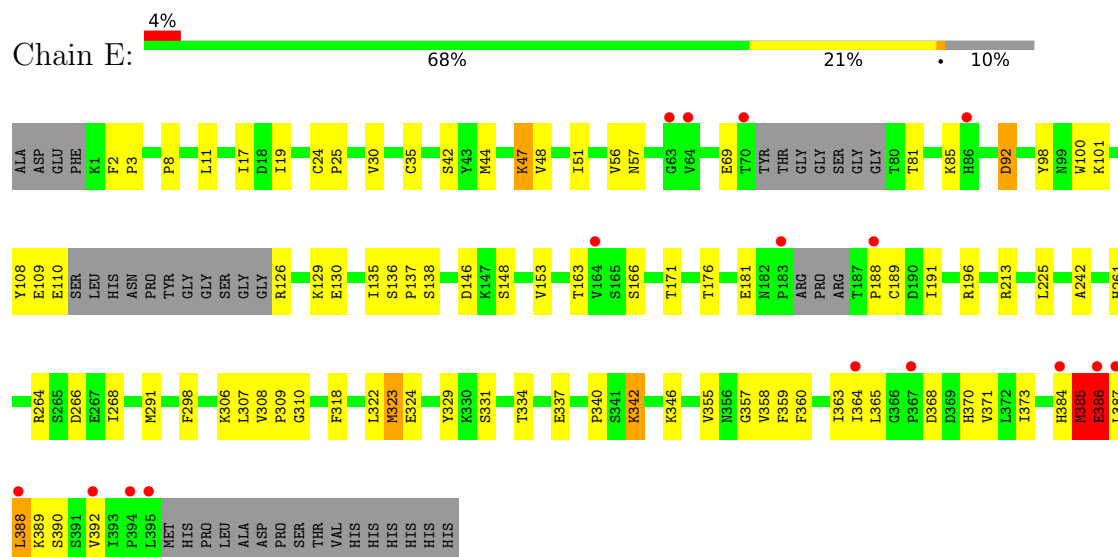
• Molecule 1: scFv 523-11



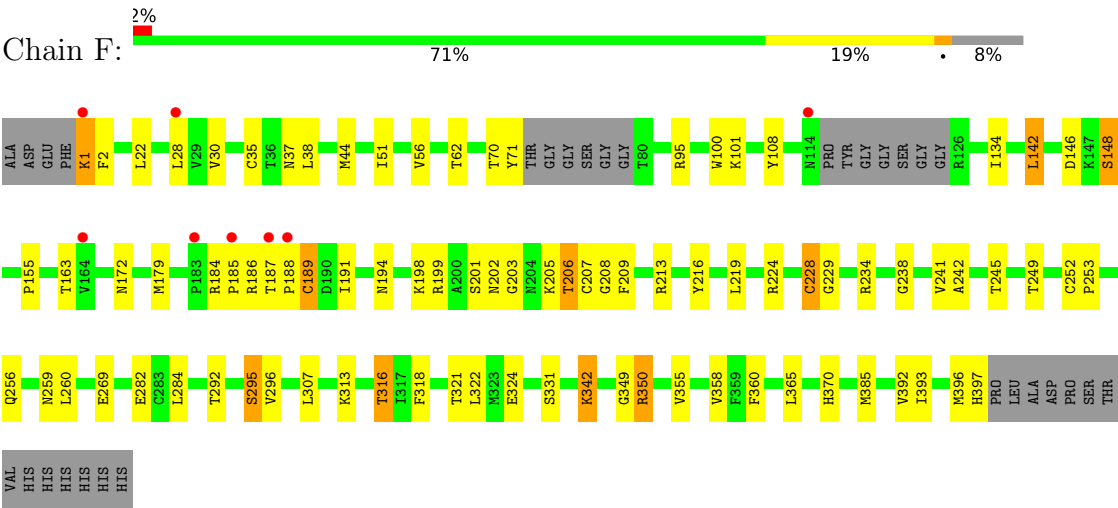
• Molecule 1: scFv 523-11



• Molecule 2: Glycoprotein



● Molecule 2: Glycoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.89Å 93.94Å 213.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.98 – 2.90 46.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.98-2.90) 99.6 (46.98-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16-3549	Depositor
R, R_{free}	0.218 , 0.268 0.219 , 0.270	Depositor DCC
R_{free} test set	1864 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	83.3	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9342	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.18	0/1761	0.42	0/2387
1	C	0.16	0/1768	0.40	0/2397
2	E	0.22	0/2970	0.51	4/4021 (0.1%)
2	F	0.35	0/3066	0.54	3/4152 (0.1%)
All	All	0.25	0/9565	0.49	7/12957 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	386	GLU	N-CA-C	13.76	126.36	111.36
2	F	342	LYS	N-CA-C	11.72	123.61	111.07
2	E	342	LYS	N-CA-C	9.70	121.54	110.97
2	F	146	ASP	N-CA-C	-6.27	99.02	109.24
2	F	295	SER	N-CA-C	5.26	118.17	109.85
2	E	385	MET	CA-C-N	5.00	127.40	120.29
2	E	385	MET	C-N-CA	5.00	127.40	120.29

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	1720	0	1643	37	0
1	C	1727	0	1652	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2902	0	2863	65	0
2	F	2993	0	2951	41	0
All	All	9342	0	9109	157	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 (157) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:386:GLU:OE2	2:E:387:LEU:CB	2.02	1.08
2:E:110:GLU:HB3	2:E:129:LYS:NZ	1.72	1.04
2:E:386:GLU:OE2	2:E:387:LEU:HB2	1.58	1.03
2:E:110:GLU:HB3	2:E:129:LYS:HZ1	1.34	0.89
2:E:342:LYS:HD2	2:E:370:HIS:CE1	2.09	0.87
2:E:44:MET:HB2	2:E:242:ALA:HB3	1.65	0.79
2:E:110:GLU:HB3	2:E:129:LYS:HZ3	1.48	0.77
2:E:386:GLU:OE2	2:E:387:LEU:HB3	1.87	0.74
2:E:110:GLU:OE2	2:E:110:GLU:HA	1.88	0.72
2:F:208:GLY:HA2	2:F:219:LEU:HG	1.72	0.71
2:E:384:HIS:O	2:E:385:MET:HB3	1.91	0.71
1:A:167:LEU:O	1:A:175:ILE:HD13	1.92	0.70
2:F:37:ASN:O	2:F:201:SER:N	2.20	0.68
2:E:163:THR:HG23	2:E:166:SER:H	1.61	0.65
1:C:82:GLU:OE1	1:C:84:ARG:NH1	2.22	0.65
2:E:69:GLU:OE1	2:E:126:ARG:NH2	2.31	0.64
1:C:6:GLN:O	1:C:111:GLN:NE2	2.30	0.64
2:E:386:GLU:OE2	2:E:387:LEU:N	2.32	0.63
2:F:313:LYS:NZ	2:F:324:GLU:OE2	2.25	0.62
1:A:17:SER:HB3	1:A:84:ARG:HE	1.63	0.62
2:F:316:THR:HG23	2:F:360:PHE:HA	1.82	0.62
2:F:234:ARG:HD3	2:F:256:GLN:HE22	1.65	0.61
2:F:44:MET:HB2	2:F:242:ALA:HB3	1.82	0.61
2:E:363:ILE:HG23	2:E:373:ILE:HG12	1.83	0.61
2:E:69:GLU:HB2	2:E:126:ARG:HD2	1.82	0.60
1:A:153:ILE:HD11	1:A:208:CYS:HB2	1.82	0.60
2:E:342:LYS:CD	2:E:370:HIS:CE1	2.83	0.60
2:E:98:TYR:OH	2:E:181:GLU:OE2	2.18	0.60
2:F:35:CYS:SG	2:F:202:ASN:HB2	2.42	0.60
1:C:100:ASN:ND2	1:C:102:ASP:OD1	2.35	0.59
2:E:298:PHE:CE1	2:E:358:VAL:HG21	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ILE:HD13	1:C:72:VAL:HG13	1.82	0.59
1:C:169:LYS:NZ	1:C:173:GLU:OE1	2.36	0.58
2:E:388:LEU:HD12	2:E:390:SER:HB2	1.86	0.58
2:E:109:GLU:OE1	2:E:109:GLU:HA	2.03	0.58
2:F:38:LEU:HD13	2:F:198:LYS:HD3	1.86	0.58
1:A:17:SER:HB3	1:A:84:ARG:NE	2.20	0.57
2:E:47:LYS:HD2	2:E:191:ILE:HA	1.87	0.56
2:E:309:PRO:HG3	2:E:331:SER:HB2	1.86	0.56
1:A:6:GLN:NE2	1:A:96:CYS:SG	2.78	0.56
2:E:3:PRO:HB3	2:E:331:SER:OG	2.05	0.56
1:A:32:TYR:HE1	1:A:101:TYR:HA	1.70	0.56
2:E:384:HIS:CG	2:E:385:MET:N	2.72	0.56
1:A:35:ASP:OD2	1:A:99:ARG:NE	2.30	0.55
2:E:92:ASP:OD1	2:E:92:ASP:N	2.23	0.55
2:F:205:LYS:HG3	2:F:206:THR:N	2.21	0.55
1:A:157:GLN:HB2	1:A:167:LEU:HD11	1.90	0.54
1:C:174:SER:C	1:C:175:ILE:HD12	2.33	0.53
1:A:39:GLN:HB2	1:A:45:LEU:HD23	1.90	0.53
2:E:358:VAL:HG23	2:E:364:ILE:HG22	1.89	0.53
2:E:334:THR:HG23	2:E:337:GLU:H	1.73	0.53
2:F:30:VAL:HG13	2:F:216:TYR:CE2	2.43	0.53
2:F:101:LYS:NZ	2:F:134:ILE:O	2.40	0.52
2:F:318:PHE:O	2:F:321:THR:HG22	2.08	0.52
1:A:102:ASP:O	2:E:346:LYS:NZ	2.34	0.52
2:E:385:MET:C	2:E:385:MET:SD	2.93	0.52
2:F:252:CYS:HB3	2:F:256:GLN:HE21	1.74	0.52
1:C:16:ALA:O	1:C:86:LEU:HD12	2.09	0.52
2:F:224:ARG:HE	2:F:249:THR:HB	1.75	0.51
2:F:342:LYS:HG3	2:F:370:HIS:CE1	2.45	0.51
1:C:175:ILE:HB	1:C:178:ILE:HD12	1.93	0.51
1:A:12:VAL:HG11	1:A:18:VAL:HB	1.91	0.51
1:A:37:VAL:HG21	1:A:109:TRP:HZ3	1.76	0.51
2:E:101:LYS:HD2	2:E:108:TYR:CE2	2.46	0.51
1:C:5:GLN:HB2	1:C:23:LYS:HB3	1.93	0.50
2:E:8:PRO:HA	2:E:329:TYR:HA	1.92	0.50
1:A:133:VAL:HG12	1:A:134:SER:H	1.77	0.50
1:A:2:VAL:HG11	1:A:108:TYR:CZ	2.47	0.50
1:A:6:GLN:HE22	1:A:96:CYS:H	1.60	0.49
2:F:185:PRO:HB2	2:F:186:ARG:HD3	1.93	0.49
2:E:384:HIS:ND1	2:E:385:MET:N	2.60	0.49
1:C:167:LEU:HA	1:C:178:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:GLN:HB2	1:C:167:LEU:HD11	1.94	0.48
2:F:253:PRO:HG2	2:F:256:GLN:HG2	1.94	0.48
1:A:209:GLN:HB2	1:A:218:PHE:CD2	2.48	0.48
2:E:171:THR:OG1	2:E:176:THR:O	2.22	0.48
2:F:1:LYS:HB3	2:F:2:PHE:H	1.52	0.48
2:E:2:PHE:CD1	2:E:3:PRO:HD2	2.49	0.48
2:E:386:GLU:OE2	2:E:387:LEU:CA	2.61	0.48
1:C:31:ASP:CG	2:F:342:LYS:HE3	2.38	0.48
2:E:213:ARG:NH2	2:E:266:ASP:OD1	2.46	0.48
1:A:175:ILE:HG22	1:A:178:ILE:HD13	1.95	0.47
2:E:318:PHE:CG	2:E:323:MET:HE1	2.50	0.47
1:A:55:TYR:OH	2:E:371:VAL:O	2.25	0.47
2:E:136:SER:O	2:E:138:SER:N	2.47	0.47
2:F:22:LEU:HD21	2:F:322:LEU:HD21	1.97	0.47
2:F:184:ARG:HB2	2:F:188:PRO:HD3	1.96	0.47
2:F:296:VAL:O	2:F:296:VAL:HG23	2.15	0.47
1:A:17:SER:CB	1:A:84:ARG:HE	2.26	0.47
2:E:386:GLU:CD	2:E:387:LEU:N	2.72	0.47
1:A:17:SER:HA	1:A:83:LEU:O	2.15	0.46
1:C:158:GLN:O	1:C:204:ALA:HB1	2.15	0.46
1:A:141:PHE:CE2	1:A:193:LEU:HD23	2.50	0.46
1:C:127:SER:HB3	1:C:142:SER:HB3	1.97	0.46
1:A:33:ASN:ND2	2:E:340:PRO:HA	2.30	0.46
2:F:349:GLY:C	2:F:350:ARG:HD2	2.41	0.46
2:F:100:TRP:HB3	2:F:108:TYR:HB2	1.98	0.46
1:A:6:GLN:NE2	1:A:110:GLY:HA3	2.30	0.46
2:F:142:LEU:HB2	2:F:148:SER:O	2.16	0.46
2:E:357:GLY:O	2:E:365:LEU:N	2.32	0.45
1:A:62:GLN:HA	1:A:65:LYS:HG3	1.99	0.45
2:F:189:CYS:O	2:F:191:ILE:N	2.48	0.45
1:A:2:VAL:HG11	1:A:108:TYR:CE2	2.52	0.45
2:E:30:VAL:HG22	2:E:308:VAL:HG11	1.99	0.45
2:E:323:MET:HB2	2:E:323:MET:HE3	1.61	0.44
1:C:53:PRO:O	1:C:74:ARG:HD2	2.16	0.44
2:F:187:THR:O	2:F:189:CYS:N	2.48	0.44
2:F:209:PHE:CZ	2:F:241:VAL:HG11	2.53	0.44
2:E:42:SER:OG	2:E:196:ARG:NH2	2.50	0.44
2:E:136:SER:HB3	2:E:137:PRO:HD3	1.99	0.44
2:E:342:LYS:HE2	2:E:368:ASP:O	2.18	0.44
2:E:69:GLU:HA	2:E:126:ARG:N	2.33	0.43
2:E:48:VAL:HG22	2:E:261:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:188:PRO:O	2:E:189:CYS:HB2	2.18	0.43
2:F:51:ILE:HG12	2:F:260:LEU:HD21	1.99	0.43
2:E:19:ILE:HG22	2:E:291:MET:HE1	1.99	0.43
2:E:390:SER:C	2:E:392:VAL:H	2.26	0.43
1:A:42:GLY:C	1:A:43:LYS:HD2	2.44	0.43
2:F:155:PRO:HA	2:F:172:ASN:OD1	2.18	0.43
2:E:130:GLU:OE2	2:F:199:ARG:HD3	2.19	0.43
2:E:389:LYS:HE3	2:E:389:LYS:HB2	1.70	0.43
2:F:70:THR:O	2:F:71:TYR:HB2	2.18	0.43
2:F:202:ASN:OD1	2:F:203:GLY:N	2.52	0.43
1:A:167:LEU:C	1:A:175:ILE:HD13	2.43	0.43
2:E:135:ILE:H	2:E:135:ILE:HD12	1.84	0.43
1:C:181:ARG:HB2	1:C:196:ASN:O	2.19	0.43
2:F:396:MET:O	2:F:397:HIS:HB2	2.20	0.42
2:E:17:ILE:HD13	2:E:324:GLU:HB3	2.00	0.42
1:C:91:THR:HG23	1:C:116:THR:HA	2.01	0.42
1:A:12:VAL:HG21	1:A:86:LEU:HD13	2.02	0.42
2:E:24:CYS:SG	2:E:25:PRO:HD2	2.59	0.42
2:F:355:VAL:O	2:F:358:VAL:HG22	2.20	0.42
2:F:95:ARG:NH2	2:F:179:MET:HE2	2.34	0.42
2:F:238:GLY:HA3	2:F:259:ASN:ND2	2.35	0.42
1:A:6:GLN:HE21	1:A:110:GLY:HA3	1.83	0.41
2:E:100:TRP:CE2	2:F:194:ASN:HB3	2.54	0.41
2:E:146:ASP:C	2:E:148:SER:H	2.28	0.41
1:A:110:GLY:O	1:A:163:SER:OG	2.37	0.41
1:A:183:SER:O	1:A:193:LEU:HD12	2.19	0.41
2:E:359:PHE:HD1	2:E:363:ILE:O	2.03	0.41
1:C:127:SER:HB3	1:C:128:PRO:HD3	2.03	0.41
1:C:38:LYS:HB2	1:C:48:ILE:HD11	2.01	0.41
2:F:187:THR:HB	2:F:188:PRO:HD3	2.02	0.41
1:A:208:CYS:O	1:A:219:GLY:N	2.54	0.41
2:E:360:PHE:O	2:E:363:ILE:HG12	2.20	0.41
2:F:228:CYS:HB3	2:F:229:GLY:H	1.69	0.41
1:A:51:ILE:HD13	1:A:72:VAL:HG13	2.03	0.41
1:A:84:ARG:HD3	1:A:85:SER:H	1.86	0.41
1:A:181:ARG:O	1:A:195:ILE:HA	2.21	0.41
2:E:2:PHE:HD1	2:E:3:PRO:HD2	1.84	0.41
1:A:133:VAL:HG12	1:A:134:SER:N	2.36	0.40
2:E:264:ARG:O	2:E:268:ILE:HG13	2.21	0.40
2:E:306:LYS:HZ3	2:E:310:GLY:HA3	1.86	0.40
2:F:206:THR:HB	2:F:219:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:51:ILE:HD13	2:E:191:ILE:HB	2.02	0.40
1:A:17:SER:HB3	1:A:84:ARG:HB2	2.03	0.40
1:C:166:LEU:O	1:C:178:ILE:HD11	2.21	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	218/228 (96%)	212 (97%)	6 (3%)	0	100	100
1	C	219/228 (96%)	211 (96%)	8 (4%)	0	100	100
2	E	360/409 (88%)	334 (93%)	25 (7%)	1 (0%)	36	65
2	F	372/409 (91%)	359 (96%)	13 (4%)	0	100	100
All	All	1169/1274 (92%)	1116 (96%)	52 (4%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	385	MET

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	188/195 (96%)	186 (99%)	2 (1%)	65	88
1	C	190/195 (97%)	189 (100%)	1 (0%)	81	93
2	E	330/361 (91%)	313 (95%)	17 (5%)	21	52
2	F	340/361 (94%)	314 (92%)	26 (8%)	12	36
All	All	1048/1112 (94%)	1002 (96%)	46 (4%)	25	59

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	MET
1	A	195	ILE
2	E	11	LEU
2	E	35	CYS
2	E	47	LYS
2	E	56	VAL
2	E	57	ASN
2	E	81	THR
2	E	85	LYS
2	E	92	ASP
2	E	153	VAL
2	E	225	LEU
2	E	307	LEU
2	E	322	LEU
2	E	323	MET
2	E	355	VAL
2	E	385	MET
2	E	386	GLU
2	E	388	LEU
1	C	65	LYS
2	F	1	LYS
2	F	28	LEU
2	F	56	VAL
2	F	62	THR
2	F	142	LEU
2	F	148	SER
2	F	163	THR
2	F	189	CYS
2	F	206	THR
2	F	207	CYS
2	F	213	ARG
2	F	228	CYS
2	F	245	THR

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Mol	Chain	Res	Type
2	F	269	GLU
2	F	282	GLU
2	F	284	LEU
2	F	292	THR
2	F	295	SER
2	F	307	LEU
2	F	316	THR
2	F	331	SER
2	F	350	ARG
2	F	365	LEU
2	F	385	MET
2	F	392	VAL
2	F	393	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	E	361	ASN
2	F	86	HIS
2	F	204	ASN
2	F	303	HIS

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	222/228 (97%)	0.02	1 (0%) 87 83	75, 114, 155, 167	0
1	C	223/228 (97%)	-0.22	0 100 100	56, 85, 126, 147	0
2	E	368/409 (89%)	0.09	16 (4%) 40 31	50, 96, 149, 195	0
2	F	378/409 (92%)	-0.05	8 (2%) 63 54	52, 86, 146, 187	0
All	All	1191/1274 (93%)	-0.03	25 (2%) 63 54	50, 93, 148, 195	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	387	LEU	5.6
2	E	388	LEU	5.2
2	E	395	LEU	3.1
2	E	386	GLU	2.9
2	E	164	VAL	2.8
2	F	1	LYS	2.8
2	E	183	PRO	2.7
2	E	63	GLY	2.6
2	E	367	PRO	2.5
2	E	384	HIS	2.5
2	E	70	THR	2.5
2	F	114	ASN	2.5
2	F	185	PRO	2.4
2	E	64	VAL	2.3
2	E	188	PRO	2.3
2	F	183	PRO	2.3
2	F	28	LEU	2.2
1	A	186	GLY	2.2
2	E	86	HIS	2.2
2	F	164	VAL	2.2
2	F	188	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	187	THR	2.1
2	E	364	ILE	2.1
2	E	394	PRO	2.0
2	E	392	VAL	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.