Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 10:08 PM JST

PDB ID	:	6LGW
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 (i) 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 (i)) were used in the production of this report:

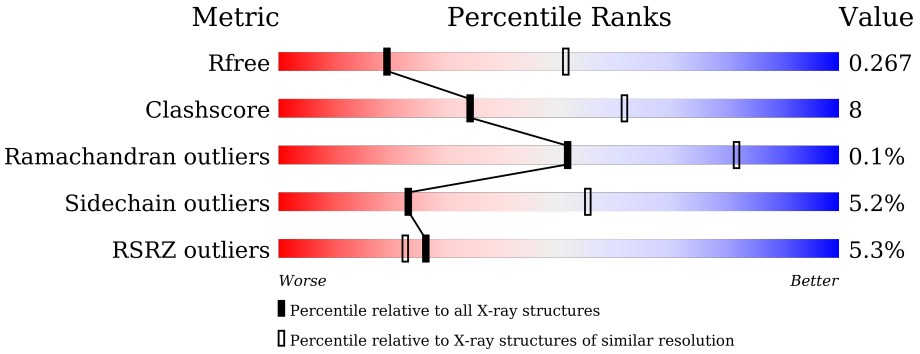
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	9% 77% 20% •
1	C	228	2% 82% 15% •
2	E	409	6% 69% 19% • 10%
2	F	409	3% 71% 19% • 8%

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
			Total	C	N	O	S			
1	A	222	1720	1085	286	342	7	0	0	0
1	C	223	1727	1088	288	344	7	0	0	0

- Molecule 2 is a protein called Glycoprotein.

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

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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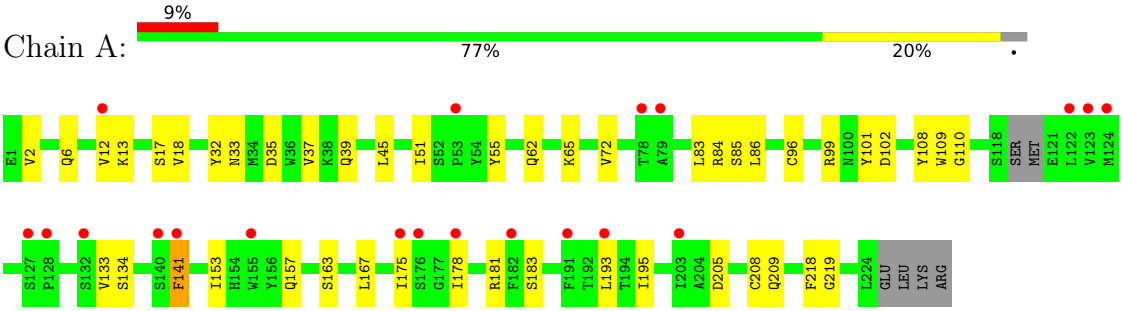
Chain	Residue	Modelled	Actual	Comment	Reference
E	408	HIS	-	expression tag	UNP D8VEC1
E	409	HIS	-	expression tag	UNP D8VEC1
E	410	HIS	-	expression tag	UNP D8VEC1
E	411	HIS	-	expression tag	UNP D8VEC1
F	-3	ALA	-	expression tag	UNP Q5JZZ2
F	-2	ASP	-	expression tag	UNP Q5JZZ2
F	-1	GLU	-	expression tag	UNP 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 (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.

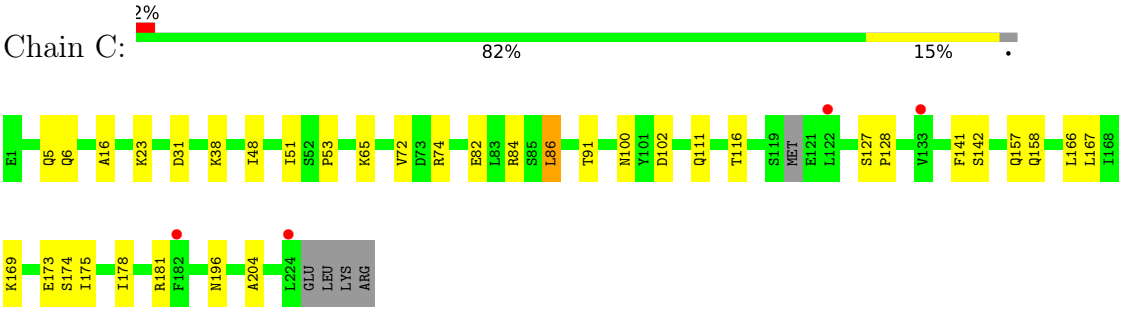
- Molecule 1: scFv 523-11

Chain A:



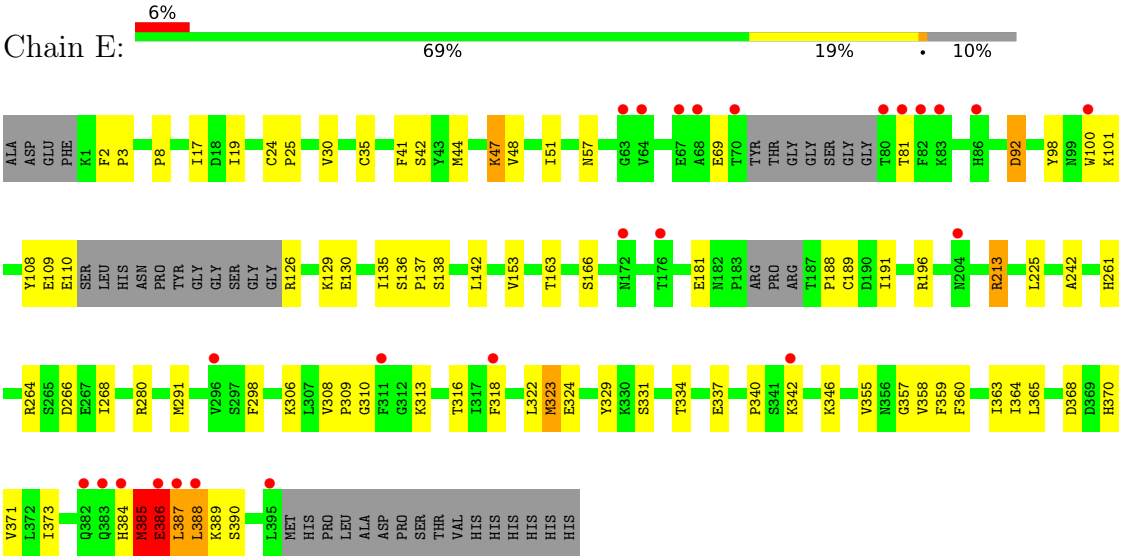
- Molecule 1: scFv 523-11

Chain C:



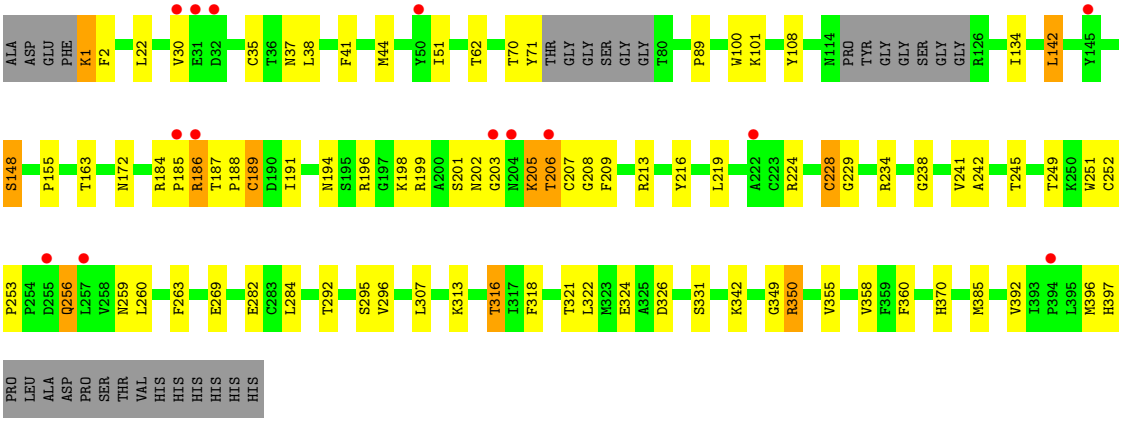
- Molecule 2: Glycoprotein

Chain E:



• Molecule 2: Glycoprotein

Chain F:



4 Data and refinement statistics (i)

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 46.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.98-2.90) 99.6 (46.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.16-3549	Depositor
R, R_{free}	0.218 , 0.268 0.218 , 0.267	Depositor DCC
R_{free} test set	1863 reflections (4.97%)	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 , 55.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.28	0/1761	0.51	0/2387
1	C	0.27	0/1768	0.51	0/2397
2	E	0.29	0/2970	0.50	1/4021 (0.0%)
2	F	0.33	0/3066	0.54	1/4152 (0.0%)
All	All	0.30	0/9565	0.52	2/12957 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	89	PRO	C-N-CA	5.96	136.59	121.70
2	E	386	GLU	N-CA-C	5.69	126.36	111.00

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	35	0
1	C	1727	0	1652	20	0
2	E	2902	0	2863	66	0
2	F	2993	0	2951	40	0
All	All	9342	0	9109	155	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 (155) 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:342:LYS:HD2	2:E:370:HIS:CE1	2.09	0.87
2:E:110:GLU:HB3	2:E:129:LYS:HZ3	1.37	0.86
2:E:110:GLU:HB3	2:E:129:LYS:HZ1	1.45	0.81
2:E:44:MET:HB2	2:E:242:ALA:HB3	1.65	0.79
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	0.73
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:110:GLU:CB	2:E:129:LYS:HZ3	2.18	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:E:318:PHE:N	2:E:323:MET:HE1	2.27	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:174:SER:C	1:C:175:ILE:HD12	2.33	0.49
1:C:167:LEU:HA	1:C:178:ILE:HD13	1.94	0.49
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:385:MET:C	2:E:385:MET:SD	2.93	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:HG23	2:F:296:VAL:O	2.15	0.47
1:A:17:SER:CB	1:A:84:ARG:HE	2.26	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: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:323:MET:HE3	2:E:323:MET:HB2	1.90	0.45
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:19:ILE:O	2:E:291:MET:HE1	2.17	0.45
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
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: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:318:PHE:H	2:E:323:MET:HE1	1.83	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
2:E:135:ILE:H	2:E:135:ILE:HD12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ARG:HB2	1:C:196:ASN:O	2.19	0.43
2:E:386:GLU:CD	2:E:387:LEU:N	2.72	0.42
1:C:31:ASP:CG	2:F:342:LYS:HE3	2.38	0.42
2:E:306:LYS:HZ3	2:E:310:GLY:HA3	1.84	0.42
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: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
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:F:349:GLY:C	2:F:350:ARG:HD2	2.41	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:316:THR:HG23	2:E:323:MET:HE3	2.03	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:F:206:THR:HB	2:F:219:LEU:HD12	2.02	0.40
2:E:51:ILE:HD13	2:E:191:ILE:HB	2.02	0.40
2:E:313:LYS:O	2:E:329:TYR:OH	2.22	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%)	41	71
2	F	372/409 (91%)	359 (96%)	13 (4%)	0	100	100
All	All	1169/1274 (92%)	1116 (96%)	52 (4%)	1 (0%)	51	82

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%)	185 (98%)	3 (2%)	62	86
1	C	190/195 (97%)	187 (98%)	3 (2%)	62	86
2	E	330/361 (91%)	312 (94%)	18 (6%)	21	53
2	F	340/361 (94%)	310 (91%)	30 (9%)	10	30
All	All	1048/1112 (94%)	994 (95%)	54 (5%)	23	55

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	141	PHE
1	A	205	ASP
2	E	35	CYS
2	E	41	PHE
2	E	47	LYS
2	E	57	ASN
2	E	81	THR
2	E	92	ASP
2	E	142	LEU
2	E	153	VAL
2	E	213	ARG
2	E	225	LEU
2	E	280	ARG
2	E	322	LEU
2	E	323	MET
2	E	355	VAL
2	E	385	MET
2	E	386	GLU
2	E	387	LEU
2	E	388	LEU
1	C	65	LYS
1	C	86	LEU
1	C	141	PHE
2	F	1	LYS
2	F	41	PHE
2	F	62	THR
2	F	142	LEU
2	F	148	SER
2	F	163	THR
2	F	186	ARG
2	F	189	CYS
2	F	196	ARG
2	F	205	LYS
2	F	206	THR
2	F	207	CYS
2	F	213	ARG
2	F	228	CYS
2	F	245	THR
2	F	251	TRP
2	F	256	GLN
2	F	263	PHE
2	F	269	GLU

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Mol	Chain	Res	Type
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	326	ASP
2	F	331	SER
2	F	350	ARG
2	F	385	MET
2	F	392	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
2	E	370	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 monosaccharides 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 (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	A	222/228 (97%)	0.52	20 (9%)	9	7	75, 114, 155, 167	0
1	C	223/228 (97%)	0.17	4 (1%)	68	67	56, 85, 126, 147	0
2	E	368/409 (89%)	0.45	25 (6%)	17	13	50, 96, 149, 195	0
2	F	378/409 (92%)	0.37	14 (3%)	41	37	52, 86, 146, 187	0
All	All	1191/1274 (93%)	0.39	63 (5%)	26	22	50, 93, 148, 195	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	387	LEU	13.8
2	F	32	ASP	8.8
2	E	388	LEU	8.2
2	E	82	PHE	7.2
2	E	386	GLU	5.6
2	E	68	ALA	4.9
2	E	80	THR	4.7
2	E	318	PHE	4.3
2	E	81	THR	4.2
2	E	86	HIS	4.2
1	A	122	LEU	4.1
2	F	185	PRO	3.9
2	E	83	LYS	3.6
1	A	191	PHE	3.6
2	E	67	GLU	3.4
2	E	384	HIS	3.4
2	F	31	GLU	3.4
2	E	63	GLY	3.3
1	A	141	PHE	3.3
2	E	64	VAL	3.2
2	F	255	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	140	SER	3.1
1	A	193	LEU	3.1
2	F	30	VAL	3.1
2	F	204	ASN	3.0
1	A	127	SER	3.0
1	A	78	THR	2.8
1	A	155	TRP	2.8
2	E	204	ASN	2.7
2	E	172	ASN	2.7
1	A	176	SER	2.7
1	A	124	MET	2.7
1	C	182	PHE	2.7
2	E	176	THR	2.7
2	F	222	ALA	2.7
1	A	128	PRO	2.7
2	F	203	GLY	2.7
1	C	224	LEU	2.6
1	A	203	ILE	2.6
2	F	145	TYR	2.6
1	A	123	VAL	2.6
1	A	79	ALA	2.6
2	E	70	THR	2.5
2	E	296	VAL	2.4
1	A	53	PRO	2.4
1	A	178	ILE	2.4
1	C	133	VAL	2.4
2	F	50	TYR	2.3
1	C	122	LEU	2.3
1	A	175	ILE	2.3
1	A	12	VAL	2.3
1	A	182	PHE	2.2
2	F	186	ARG	2.2
2	E	100	TRP	2.2
2	F	206	THR	2.2
1	A	132	SER	2.1
2	E	382	GLN	2.1
2	E	395	LEU	2.1
2	F	257	LEU	2.1
2	E	311	PHE	2.1
2	E	383	GLN	2.0
2	F	394	PRO	2.0
2	E	342	LYS	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 monosaccharides 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.