



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:21 PM UTC

PDB ID : 9VDY / pdb_00009vdy
Title : hA5-6 Fab bound to SFTSV glycoprotein Gn
Authors : Deng, Z.; Kuang, W.; Zhao, H.
Deposited on : 2025-06-09
Resolution : 2.28 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

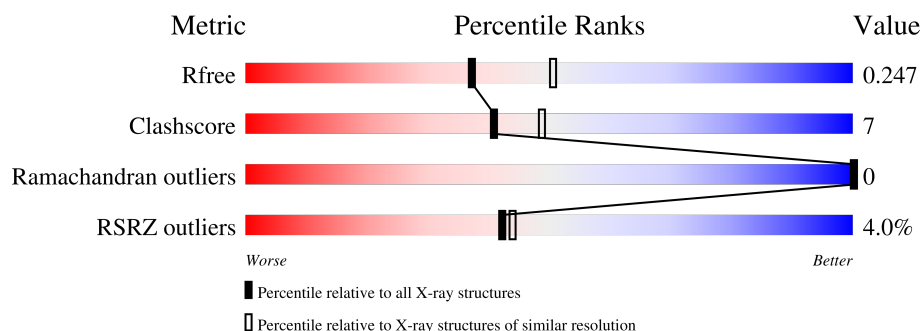
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	338	3% 81% 12% 7%
1	B	338	3% 85% 7% 7%
2	C	232	6% 75% 18% 8%
2	H	232	6% 75% 17% 8%
3	D	218	% 85% 13% .
3	L	218	4% 83% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11591 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 Envelopment polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2410	1510	417	457	26			
1	B	314	Total	C	N	O	S	0	0	0
			2410	1510	417	457	26			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	GLY	-	expression tag	UNP W5VWE0
A	342	SER	-	expression tag	UNP W5VWE0
A	343	THR	-	expression tag	UNP W5VWE0
A	344	LEU	-	expression tag	UNP W5VWE0
A	345	GLU	-	expression tag	UNP W5VWE0
A	346	VAL	-	expression tag	UNP W5VWE0
A	347	LEU	-	expression tag	UNP W5VWE0
A	348	PHE	-	expression tag	UNP W5VWE0
A	349	GLN	-	expression tag	UNP W5VWE0
A	350	GLY	-	expression tag	UNP W5VWE0
A	351	PRO	-	expression tag	UNP W5VWE0
A	352	HIS	-	expression tag	UNP W5VWE0
A	353	HIS	-	expression tag	UNP W5VWE0
A	354	HIS	-	expression tag	UNP W5VWE0
A	355	HIS	-	expression tag	UNP W5VWE0
A	356	HIS	-	expression tag	UNP W5VWE0
A	357	HIS	-	expression tag	UNP W5VWE0
B	341	GLY	-	expression tag	UNP W5VWE0
B	342	SER	-	expression tag	UNP W5VWE0
B	343	THR	-	expression tag	UNP W5VWE0
B	344	LEU	-	expression tag	UNP W5VWE0
B	345	GLU	-	expression tag	UNP W5VWE0
B	346	VAL	-	expression tag	UNP W5VWE0
B	347	LEU	-	expression tag	UNP W5VWE0
B	348	PHE	-	expression tag	UNP W5VWE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	349	GLN	-	expression tag	UNP W5VWE0
B	350	GLY	-	expression tag	UNP W5VWE0
B	351	PRO	-	expression tag	UNP W5VWE0
B	352	HIS	-	expression tag	UNP W5VWE0
B	353	HIS	-	expression tag	UNP W5VWE0
B	354	HIS	-	expression tag	UNP W5VWE0
B	355	HIS	-	expression tag	UNP W5VWE0
B	356	HIS	-	expression tag	UNP W5VWE0
B	357	HIS	-	expression tag	UNP W5VWE0

- Molecule 2 is a protein called hA5-6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1615	1021	266	321	7			
2	H	214	Total	C	N	O	S	0	0	0
			1615	1021	266	321	7			

- Molecule 3 is a protein called hA5-6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	215	Total	C	N	O	S	0	0	0
			1644	1027	273	339	5			
3	L	215	Total	C	N	O	S	0	0	0
			1644	1027	273	339	5			

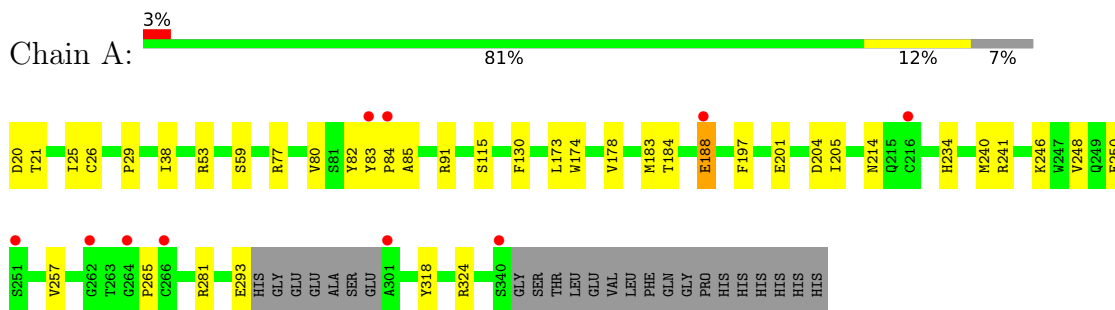
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	B	78	Total	O	0	0
			78	78		
4	C	30	Total	O	0	0
			30	30		
4	D	23	Total	O	0	0
			23	23		
4	H	20	Total	O	0	0
			20	20		
4	L	28	Total	O	0	0
			28	28		

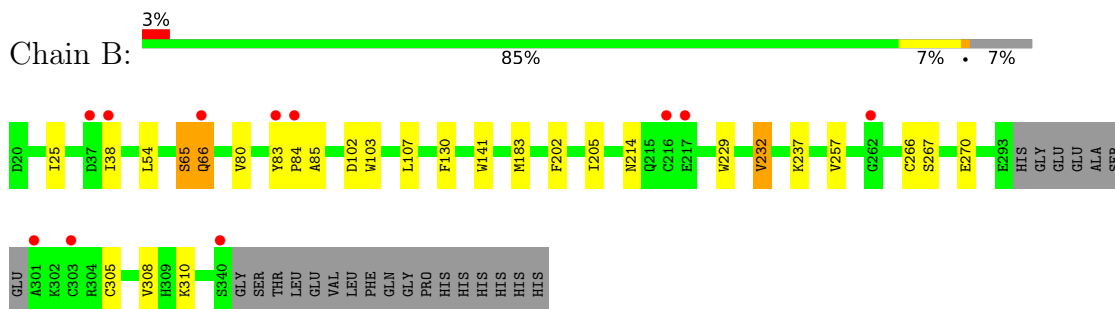
3 Residue-property plots [i](#)

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.

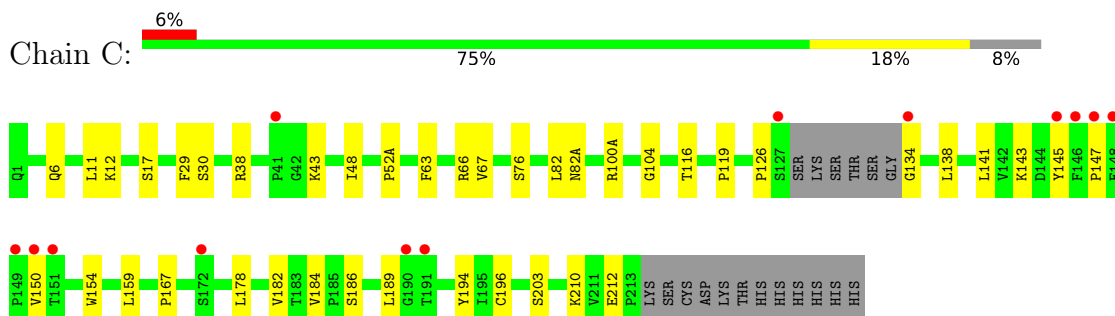
- Molecule 1: Envelopment polypeptide



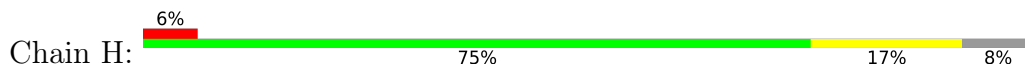
- Molecule 1: Envelopment polypeptide

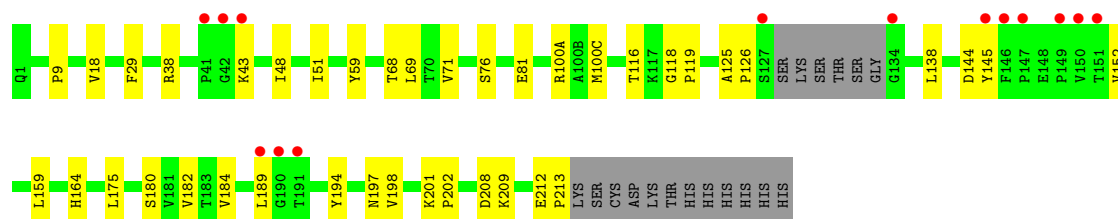


- Molecule 2: hA5-6 Fab heavy chain

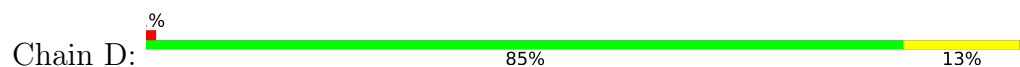


- Molecule 2: hA5-6 Fab heavy chain

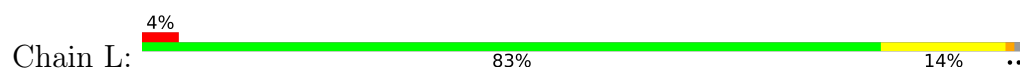




• Molecule 3: hA5-6 Fab light chain



• Molecule 3: hA5-6 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.96Å 91.11Å 308.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 2.28 29.93 – 2.28	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.93-2.28) 99.9 (29.93-2.28)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.204 , 0.240 (Not available) , 0.247	Depositor DCC
R_{free} test set	4262 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11591	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.29% 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	0.50	0/2470	0.76	2/3332 (0.1%)
1	B	0.51	0/2470	0.79	5/3332 (0.2%)
2	C	0.55	0/1655	0.76	0/2253
2	H	0.58	1/1655 (0.1%)	0.78	3/2253 (0.1%)
3	D	0.52	1/1678 (0.1%)	0.76	2/2280 (0.1%)
3	L	0.55	1/1678 (0.1%)	0.80	3/2280 (0.1%)
All	All	0.53	3/11606 (0.0%)	0.78	15/15730 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	118	GLY	C-N	13.57	1.50	1.33
3	D	112	ALA	C-N	12.52	1.49	1.33
3	L	112	ALA	C-N	12.27	1.49	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	112	ALA	CA-C-N	13.65	133.41	119.76
3	L	112	ALA	C-N-CA	13.65	133.41	119.76
3	D	112	ALA	CA-C-N	13.38	133.36	119.85
3	D	112	ALA	C-N-CA	13.38	133.36	119.85
2	H	118	GLY	CA-C-N	11.48	133.17	120.66
2	H	118	GLY	C-N-CA	11.48	133.17	120.66
1	B	66	GLN	N-CA-CB	-9.68	97.75	112.47
1	B	84	PRO	N-CA-C	-7.47	97.08	112.47
1	A	84	PRO	N-CA-C	-7.44	97.15	112.47
1	B	65	SER	CA-C-N	-7.11	112.50	122.74
1	B	65	SER	C-N-CA	-7.11	112.50	122.74
3	L	108	ARG	N-CA-CB	-5.83	102.35	111.56
1	A	188	GLU	CA-CB-CG	5.39	124.89	114.10
2	H	116	THR	CB-CA-C	-5.21	100.73	109.65
1	B	232	VAL	CG1-CB-CG2	-5.11	99.56	110.80

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	2410	0	2311	30	0
1	B	2410	0	2311	20	0
2	C	1615	0	1573	28	0
2	H	1615	0	1573	27	0
3	D	1644	0	1589	24	0
3	L	1644	0	1589	22	0
4	A	74	0	0	2	0
4	B	78	0	0	0	0
4	C	30	0	0	1	0
4	D	23	0	0	0	0
4	H	20	0	0	1	0
4	L	28	0	0	2	0
All	All	11591	0	10946	145	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 7.

All (145) 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:266:CYS:HB3	1:B:270:GLU:HG3	1.60	0.84
2:C:126:PRO:HG3	2:C:138:LEU:HB3	1.63	0.80
1:B:65:SER:O	1:B:66:GLN:HB2	1.82	0.77
3:L:99:GLY:O	4:L:301:HOH:O	2.03	0.75
2:C:17:SER:OG	2:C:82(A):ASN:HB3	1.87	0.74
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.69	0.73
1:A:178:VAL:O	4:A:401:HOH:O	2.06	0.73
1:B:202:PHE:HB3	1:B:205:ILE:HD12	1.70	0.72
3:L:183:LYS:HE2	3:L:187:GLU:OE2	1.91	0.69
1:A:20:ASP:HB3	1:A:91:ARG:HH22	1.57	0.69
1:A:188:GLU:HB3	1:A:234:HIS:CE1	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.76	0.68
2:C:178:LEU:C	2:C:178:LEU:HD12	2.19	0.68
2:C:210:LYS:NZ	2:C:212:GLU:OE1	2.26	0.68
3:L:24:LYS:HD3	3:L:70:ASP:OD2	1.94	0.67
3:L:61:ARG:HG3	3:L:75:ILE:HG23	1.76	0.67
1:A:25:ILE:HD11	1:A:257:VAL:HB	1.77	0.66
2:C:119:PRO:HB3	2:C:145:TYR:HB3	1.77	0.65
2:C:100(A):ARG:HG2	3:D:91:SER:HB2	1.77	0.64
2:H:100(A):ARG:HG2	3:L:91:SER:HB2	1.80	0.63
3:D:37:GLN:HB2	3:D:47:LEU:HD11	1.82	0.61
2:H:126:PRO:HG2	2:H:189:LEU:HD11	1.81	0.61
2:C:167:PRO:HG2	3:D:162:SER:OG	2.01	0.61
3:L:166:GLN:HG3	3:L:173:TYR:CZ	2.36	0.60
3:D:112:ALA:HB2	3:D:200:GLY:O	2.02	0.60
2:H:68:THR:O	4:H:301:HOH:O	2.15	0.60
3:L:61:ARG:NH2	4:L:302:HOH:O	2.34	0.60
2:C:63:PHE:HB3	2:C:67:VAL:CG2	2.32	0.60
3:L:147:GLN:HB3	3:L:195:GLU:HB3	1.82	0.60
2:H:126:PRO:HG3	2:H:138:LEU:HB3	1.83	0.60
3:D:211:ARG:HG2	3:D:211:ARG:HH11	1.67	0.59
3:L:112:ALA:HB2	3:L:200:GLY:O	2.03	0.59
1:B:83:TYR:O	1:B:85:ALA:N	2.36	0.58
2:H:43:LYS:HB3	2:H:43:LYS:NZ	2.18	0.58
3:D:123:GLU:OE1	3:D:123:GLU:N	2.22	0.58
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.86	0.58
3:L:151:ASP:OD1	3:L:190:LYS:HB3	2.04	0.58
2:C:63:PHE:HB3	2:C:67:VAL:HG23	1.85	0.57
1:B:232:VAL:HG22	1:B:232:VAL:O	2.05	0.56
2:C:67:VAL:HG22	2:C:82:LEU:HD13	1.86	0.56
2:H:51:ILE:HD13	2:H:71:VAL:HG13	1.86	0.56
1:A:205:ILE:O	1:A:214:ASN:HB2	2.05	0.56
1:B:232:VAL:O	1:B:232:VAL:CG2	2.53	0.56
1:B:267:SER:OG	1:B:270:GLU:HG2	2.05	0.56
2:C:154:TRP:CH2	2:C:196:CYS:HB3	2.41	0.56
3:L:145:LYS:HB3	3:L:197:THR:HB	1.86	0.56
2:C:43:LYS:NZ	4:C:302:HOH:O	2.36	0.56
2:C:150:VAL:CG2	2:C:178:LEU:HD21	2.36	0.56
1:B:83:TYR:C	1:B:83:TYR:CD1	2.84	0.55
3:D:147:GLN:HB3	3:D:195:GLU:HB3	1.89	0.55
1:A:201:GLU:O	1:A:241:ARG:NH2	2.37	0.54
1:A:250:GLU:OE2	1:A:324:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:THR:HG22	1:A:324:ARG:HD2	1.89	0.54
2:H:100(C):MET:HE1	3:L:98:PHE:HZ	1.73	0.54
1:A:83:TYR:CD1	1:A:83:TYR:C	2.84	0.54
1:A:184:THR:CG2	1:A:324:ARG:HB3	2.38	0.54
3:D:60:ASP:N	3:D:60:ASP:OD1	2.39	0.54
1:A:83:TYR:O	1:A:85:ALA:N	2.41	0.53
1:A:38:ILE:HD11	1:A:59:SER:HB2	1.89	0.53
2:H:29:PHE:CD2	2:H:76:SER:HA	2.43	0.53
1:A:21:THR:OG1	1:A:91:ARG:NH1	2.42	0.52
2:C:38:ARG:HB3	2:C:48:ILE:HD11	1.92	0.52
1:A:115:SER:O	4:A:402:HOH:O	2.19	0.52
1:B:205:ILE:O	1:B:214:ASN:HB2	2.10	0.52
3:D:13:VAL:HG21	3:D:19:ALA:HB2	1.91	0.52
3:D:110:VAL:HG21	3:D:199:GLN:NE2	2.24	0.51
3:D:182:SER:OG	3:D:185:ASP:HB2	2.11	0.51
1:B:183:MET:HE1	1:B:232:VAL:HA	1.94	0.50
3:L:122:ASP:O	3:L:126:LYS:HG2	2.11	0.50
3:L:125:LEU:O	3:L:183:LYS:HD2	2.12	0.50
2:H:9:PRO:HG2	2:H:202:PRO:HD3	1.94	0.49
3:L:154:LEU:HD12	3:L:155:GLN:N	2.27	0.49
1:B:308:VAL:HG23	1:B:310:LYS:HG2	1.95	0.49
3:D:121:SER:HB2	3:D:123:GLU:OE1	2.13	0.49
3:D:110:VAL:HG21	3:D:199:GLN:HE21	1.77	0.48
2:H:144:ASP:HB3	2:H:175:LEU:HD13	1.95	0.48
3:D:81:GLU:H	3:D:81:GLU:CD	2.13	0.48
3:D:187:GLU:O	3:D:211:ARG:NH2	2.45	0.48
2:C:159:LEU:HD21	2:C:182:VAL:HG21	1.95	0.48
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.50	0.47
2:H:197:ASN:ND2	2:H:208:ASP:OD1	2.23	0.46
3:L:81:GLU:H	3:L:81:GLU:CD	2.23	0.46
1:A:240:MET:HG2	1:A:318:TYR:CE1	2.50	0.46
3:D:143:GLU:H	3:D:143:GLU:CD	2.24	0.46
1:B:38:ILE:HG13	1:B:38:ILE:O	2.15	0.46
2:C:11:LEU:HB2	2:C:147:PRO:HG3	1.98	0.46
2:C:184:VAL:HG11	2:C:194:TYR:CZ	2.51	0.46
2:H:126:PRO:CG	2:H:189:LEU:HD11	2.46	0.46
2:C:66:ARG:HD2	2:C:82(A):ASN:O	2.16	0.46
2:H:212:GLU:HB2	2:H:213:PRO:HD2	1.98	0.45
1:B:38:ILE:HD11	1:B:103:TRP:HH2	1.81	0.45
1:B:65:SER:O	1:B:66:GLN:CB	2.52	0.45
2:H:159:LEU:HD21	2:H:182:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:HD11	1:B:257:VAL:HB	1.97	0.45
2:C:30:SER:HA	2:C:52(A):PRO:HB2	1.98	0.45
3:D:190:LYS:HG2	3:D:191:VAL:HG23	1.99	0.45
3:D:211:ARG:HG2	3:D:211:ARG:NH1	2.32	0.45
2:H:152:VAL:HG11	2:H:180:SER:CB	2.47	0.45
1:A:82:TYR:HA	1:A:174:TRP:O	2.17	0.45
3:D:147:GLN:HG3	3:D:154:LEU:CD1	2.47	0.45
1:A:29:PRO:HD3	1:A:53:ARG:HA	1.99	0.44
1:B:229:TRP:CE3	1:B:237:LYS:HD3	2.51	0.44
2:H:164:HIS:HE1	3:L:138:ASN:OD1	2.01	0.44
1:A:38:ILE:CD1	1:A:59:SER:HB2	2.47	0.44
2:C:134:GLY:O	2:C:186:SER:OG	2.36	0.44
3:D:14:SER:HB2	3:D:17:GLU:HG3	2.00	0.44
2:H:100(C):MET:HE3	2:H:100(C):MET:HB2	1.86	0.44
1:B:102:ASP:HA	1:B:107:LEU:O	2.18	0.43
3:D:120:PRO:HD3	3:D:132:VAL:HG22	2.00	0.43
1:A:26:CYS:SG	1:A:265:PRO:HD3	2.58	0.43
1:B:257:VAL:O	1:B:305:CYS:HA	2.18	0.43
2:C:29:PHE:CD2	2:C:76:SER:HA	2.54	0.43
3:D:112:ALA:HB2	3:D:200:GLY:C	2.44	0.43
3:D:81:GLU:OE1	3:D:81:GLU:N	2.33	0.42
1:A:246:LYS:HD3	1:A:248:VAL:CG2	2.49	0.42
2:C:178:LEU:C	2:C:178:LEU:CD1	2.90	0.42
2:H:100(C):MET:HE1	3:L:98:PHE:CZ	2.52	0.42
2:C:189:LEU:HD12	2:C:189:LEU:HA	1.87	0.42
1:A:250:GLU:HA	1:A:250:GLU:OE1	2.18	0.42
1:A:183:MET:HE3	1:A:183:MET:HB2	1.78	0.42
2:C:11:LEU:O	2:C:12:LYS:HD2	2.20	0.42
1:A:204:ASP:OD1	1:A:204:ASP:N	2.38	0.42
3:D:184:ALA:O	3:D:188:LYS:HG3	2.19	0.42
2:H:18:VAL:O	2:H:81:GLU:HA	2.19	0.42
2:C:6:GLN:OE1	2:C:104:GLY:HA3	2.20	0.42
1:A:184:THR:HG23	1:A:324:ARG:HB3	2.01	0.41
1:A:38:ILE:HG21	1:A:38:ILE:HD13	1.49	0.41
2:C:141:LEU:HD22	2:C:141:LEU:HA	1.89	0.41
3:L:119:PRO:HB3	3:L:209:PHE:CE2	2.55	0.41
2:C:141:LEU:CD1	2:C:143:LYS:HB2	2.51	0.41
2:H:152:VAL:HG22	2:H:198:VAL:HG22	2.02	0.41
1:A:25:ILE:HD13	1:A:25:ILE:HG21	1.79	0.41
2:H:59:TYR:HE1	2:H:69:LEU:HG	1.85	0.41
1:A:130:PHE:HA	1:A:173:LEU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HD11	1:B:80:VAL:HG12	2.03	0.41
1:B:130:PHE:CE1	1:B:141:TRP:CE3	3.09	0.41
2:H:209:LYS:HB2	2:H:209:LYS:HE2	1.81	0.41
3:L:108:ARG:NH1	3:L:170:ASP:O	2.54	0.41
1:A:197:PHE:HD1	1:A:318:TYR:CZ	2.40	0.40
2:C:116:THR:HG22	2:C:203:SER:HB3	2.04	0.40
1:A:77:ARG:O	1:A:80:VAL:HG13	2.21	0.40
1:A:281:ARG:NH1	1:A:293:GLU:O	2.55	0.40
2:H:125:ALA:HA	2:H:126:PRO:HD3	1.93	0.40
2:H:201:LYS:N	2:H:202:PRO:HD2	2.36	0.40
3:L:143:GLU:N	3:L:143:GLU:CD	2.80	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	310/338 (92%)	303 (98%)	7 (2%)	0	100	100
1	B	310/338 (92%)	302 (97%)	8 (3%)	0	100	100
2	C	210/232 (90%)	205 (98%)	5 (2%)	0	100	100
2	H	210/232 (90%)	203 (97%)	7 (3%)	0	100	100
3	D	213/218 (98%)	209 (98%)	4 (2%)	0	100	100
3	L	213/218 (98%)	208 (98%)	5 (2%)	0	100	100
All	All	1466/1576 (93%)	1430 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	314/338 (92%)	0.19	10 (3%) 50 52	38, 52, 70, 94	0
1	B	314/338 (92%)	0.18	11 (3%) 47 49	38, 51, 72, 93	0
2	C	214/232 (92%)	0.39	13 (6%) 27 28	43, 58, 90, 99	0
2	H	214/232 (92%)	0.49	14 (6%) 25 26	43, 61, 87, 99	0
3	D	215/218 (98%)	0.37	3 (1%) 73 75	46, 61, 75, 90	0
3	L	215/218 (98%)	0.43	8 (3%) 45 47	44, 62, 77, 85	0
All	All	1486/1576 (94%)	0.32	59 (3%) 42 44	38, 57, 78, 99	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	146	PHE	6.0
2	C	145	TYR	5.3
1	A	301	ALA	5.2
2	H	145	TYR	5.1
2	H	146	PHE	5.0
2	C	150	VAL	4.9
2	C	147	PRO	4.8
2	H	150	VAL	4.7
2	C	149	PRO	4.3
2	C	191	THR	4.0
2	H	147	PRO	3.9
2	H	191	THR	3.9
2	H	42	GLY	3.7
2	H	151	THR	3.7
1	B	217	GLU	3.6
1	B	301	ALA	3.5
2	H	149	PRO	3.5
2	H	41	PRO	3.4
2	H	190	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	C	151	THR	3.3
1	B	66	GLN	3.3
3	L	185	ASP	3.2
2	C	148	GLU	3.0
1	A	340	SER	3.0
1	A	83	TYR	3.0
1	B	216	CYS	2.9
2	H	134	GLY	2.9
1	B	262	GLY	2.8
2	H	127	SER	2.8
2	C	127	SER	2.8
1	B	84	PRO	2.7
1	B	83	TYR	2.6
1	B	340	SER	2.6
2	H	43	LYS	2.6
1	A	188	GLU	2.6
2	C	190	GLY	2.6
2	H	189	LEU	2.5
3	D	185	ASP	2.5
3	L	203	SER	2.5
3	L	94	ASP	2.3
2	C	134	GLY	2.3
1	A	264	GLY	2.2
1	B	38	ILE	2.2
3	L	194	CYS	2.2
1	B	303	CYS	2.2
1	A	262	GLY	2.1
1	A	216	CYS	2.1
2	C	172	SER	2.1
1	A	266	CYS	2.1
3	L	13	VAL	2.1
1	A	251	SER	2.1
3	D	19	ALA	2.1
1	A	84	PRO	2.1
2	C	41	PRO	2.1
3	L	169	LYS	2.0
3	D	203	SER	2.0
1	B	37	ASP	2.0
3	L	184	ALA	2.0
3	L	183	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 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.