



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2025 – 01:07 pm BST

PDB ID : 9HNG / pdb_00009hng
Title : Structure of A16/G9 (G9 mutant - H44Y) of Vaccinia virus in complex with VHH D07
Authors : Vernuccio, R.; Meola, A.; Guardado-Calvo, P.
Deposited on : 2024-12-10
Resolution : 2.50 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

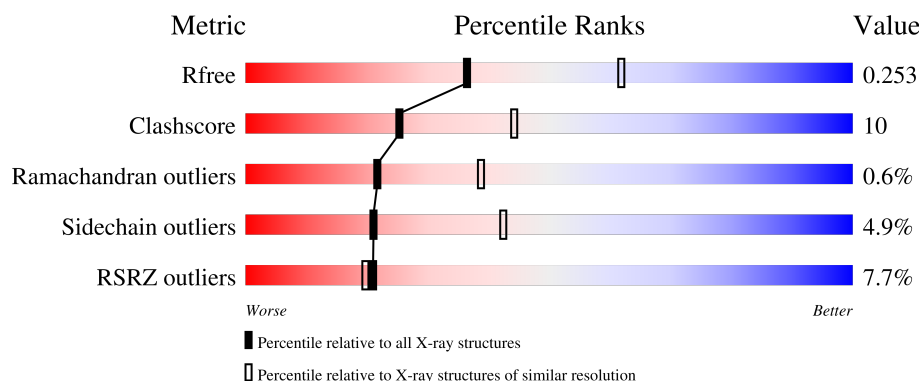
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	358	<div> <div>9%</div> <div>55%</div> <div>23%</div> <div>•</div> <div>19%</div> </div>
2	B	334	<div> <div>4%</div> <div>67%</div> <div>12%</div> <div>•</div> <div>20%</div> </div>
3	J000	154	<div> <div>5%</div> <div>73%</div> <div>•</div> <div>23%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5512 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 Virion membrane protein OPG143.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2379	1509	408	439	23	0	0	0

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP P16710
A	-17	LYS	-	expression tag	UNP P16710
A	-16	LEU	-	expression tag	UNP P16710
A	-15	CYS	-	expression tag	UNP P16710
A	-14	ILE	-	expression tag	UNP P16710
A	-13	LEU	-	expression tag	UNP P16710
A	-12	LEU	-	expression tag	UNP P16710
A	-11	ALA	-	expression tag	UNP P16710
A	-10	VAL	-	expression tag	UNP P16710
A	-9	VAL	-	expression tag	UNP P16710
A	-8	ALA	-	expression tag	UNP P16710
A	-7	PHE	-	expression tag	UNP P16710
A	-6	VAL	-	expression tag	UNP P16710
A	-5	GLY	-	expression tag	UNP P16710
A	-4	LEU	-	expression tag	UNP P16710
A	-3	SER	-	expression tag	UNP P16710
A	-2	LEU	-	expression tag	UNP P16710
A	-1	GLY	-	expression tag	UNP P16710
A	0	ARG	-	expression tag	UNP P16710
A	1	SER	-	expression tag	UNP P16710
A	2	ALA	-	expression tag	UNP P16710
A	296	GLY	-	expression tag	UNP P16710
A	297	SER	-	expression tag	UNP P16710
A	298	GLY	-	expression tag	UNP P16710
A	299	LEU	-	expression tag	UNP P16710
A	300	VAL	-	expression tag	UNP P16710
A	301	PRO	-	expression tag	UNP P16710

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Chain	Residue	Modelled	Actual	Comment	Reference
A	302	ARG	-	expression tag	UNP P16710
A	303	GLY	-	expression tag	UNP P16710
A	304	SER	-	expression tag	UNP P16710
A	305	GLY	-	expression tag	UNP P16710
A	306	GLY	-	expression tag	UNP P16710
A	307	SER	-	expression tag	UNP P16710
A	308	GLY	-	expression tag	UNP P16710
A	309	GLY	-	expression tag	UNP P16710
A	310	SER	-	expression tag	UNP P16710
A	311	HIS	-	expression tag	UNP P16710
A	312	HIS	-	expression tag	UNP P16710
A	313	HIS	-	expression tag	UNP P16710
A	314	HIS	-	expression tag	UNP P16710
A	315	HIS	-	expression tag	UNP P16710
A	316	HIS	-	expression tag	UNP P16710
A	317	HIS	-	expression tag	UNP P16710
A	318	HIS	-	expression tag	UNP P16710
A	319	GLY	-	expression tag	UNP P16710
A	320	GLY	-	expression tag	UNP P16710
A	321	SER	-	expression tag	UNP P16710
A	322	GLY	-	expression tag	UNP P16710
A	323	THR	-	expression tag	UNP P16710
A	324	GLY	-	expression tag	UNP P16710
A	325	GLY	-	expression tag	UNP P16710
A	326	LEU	-	expression tag	UNP P16710
A	327	ASN	-	expression tag	UNP P16710
A	328	ASP	-	expression tag	UNP P16710
A	329	ILE	-	expression tag	UNP P16710
A	330	PHE	-	expression tag	UNP P16710
A	331	GLU	-	expression tag	UNP P16710
A	332	ALA	-	expression tag	UNP P16710
A	333	GLN	-	expression tag	UNP P16710
A	334	LYS	-	expression tag	UNP P16710
A	335	ILE	-	expression tag	UNP P16710
A	336	GLU	-	expression tag	UNP P16710
A	337	TRP	-	expression tag	UNP P16710
A	338	HIS	-	expression tag	UNP P16710
A	339	GLU	-	expression tag	UNP P16710

- Molecule 2 is a protein called Entry-fusion complex protein OPG094.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	267	Total	C	N	O	S	0	0	0
			2153	1348	380	408	17			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP P07611
B	-15	LYS	-	expression tag	UNP P07611
B	-14	LEU	-	expression tag	UNP P07611
B	-13	CYS	-	expression tag	UNP P07611
B	-12	ILE	-	expression tag	UNP P07611
B	-11	LEU	-	expression tag	UNP P07611
B	-10	LEU	-	expression tag	UNP P07611
B	-9	ALA	-	expression tag	UNP P07611
B	-8	VAL	-	expression tag	UNP P07611
B	-7	VAL	-	expression tag	UNP P07611
B	-6	ALA	-	expression tag	UNP P07611
B	-5	PHE	-	expression tag	UNP P07611
B	-4	VAL	-	expression tag	UNP P07611
B	-3	GLY	-	expression tag	UNP P07611
B	-2	LEU	-	expression tag	UNP P07611
B	-1	SER	-	expression tag	UNP P07611
B	0	LEU	-	expression tag	UNP P07611
B	1	GLY	-	expression tag	UNP P07611
B	2	ALA	-	expression tag	UNP P07611
B	44	TYR	HIS	engineered mutation	UNP P07611
B	82	ALA	ASN	conflict	UNP P07611
B	93	GLN	ASN	conflict	UNP P07611
B	159	ALA	THR	conflict	UNP P07611
B	272	GLY	-	expression tag	UNP P07611
B	273	SER	-	expression tag	UNP P07611
B	274	GLY	-	expression tag	UNP P07611
B	275	LEU	-	expression tag	UNP P07611
B	276	VAL	-	expression tag	UNP P07611
B	277	PRO	-	expression tag	UNP P07611
B	278	ARG	-	expression tag	UNP P07611
B	279	GLY	-	expression tag	UNP P07611
B	280	SER	-	expression tag	UNP P07611
B	281	LEU	-	expression tag	UNP P07611
B	282	GLU	-	expression tag	UNP P07611
B	283	ASP	-	expression tag	UNP P07611
B	284	ASP	-	expression tag	UNP P07611
B	285	ASP	-	expression tag	UNP P07611

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Chain	Residue	Modelled	Actual	Comment	Reference
B	286	ASP	-	expression tag	UNP P07611
B	287	LYS	-	expression tag	UNP P07611
B	288	ALA	-	expression tag	UNP P07611
B	289	GLY	-	expression tag	UNP P07611
B	290	TRP	-	expression tag	UNP P07611
B	291	SER	-	expression tag	UNP P07611
B	292	HIS	-	expression tag	UNP P07611
B	293	PRO	-	expression tag	UNP P07611
B	294	GLN	-	expression tag	UNP P07611
B	295	PHE	-	expression tag	UNP P07611
B	296	GLU	-	expression tag	UNP P07611
B	297	LYS	-	expression tag	UNP P07611
B	298	GLY	-	expression tag	UNP P07611
B	299	GLY	-	expression tag	UNP P07611
B	300	GLY	-	expression tag	UNP P07611
B	301	SER	-	expression tag	UNP P07611
B	302	GLY	-	expression tag	UNP P07611
B	303	GLY	-	expression tag	UNP P07611
B	304	GLY	-	expression tag	UNP P07611
B	305	SER	-	expression tag	UNP P07611
B	306	GLY	-	expression tag	UNP P07611
B	307	GLY	-	expression tag	UNP P07611
B	308	GLY	-	expression tag	UNP P07611
B	309	SER	-	expression tag	UNP P07611
B	310	TRP	-	expression tag	UNP P07611
B	311	SER	-	expression tag	UNP P07611
B	312	HIS	-	expression tag	UNP P07611
B	313	PRO	-	expression tag	UNP P07611
B	314	GLN	-	expression tag	UNP P07611
B	315	PHE	-	expression tag	UNP P07611
B	316	GLU	-	expression tag	UNP P07611
B	317	LYS	-	expression tag	UNP P07611

- Molecule 3 is a protein called VHH D07.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J000	118	Total	C	N	O	S	0	0	0
			897	553	162	177	5			

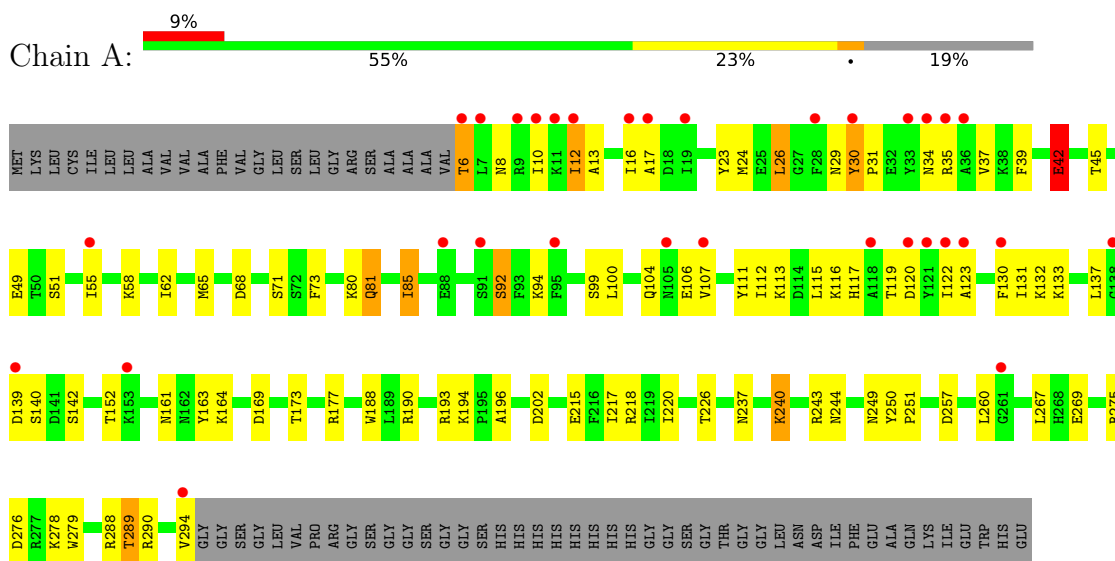
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	57	Total 57	O 57	0	0
4	J000	3	Total 3	O 3	0	0

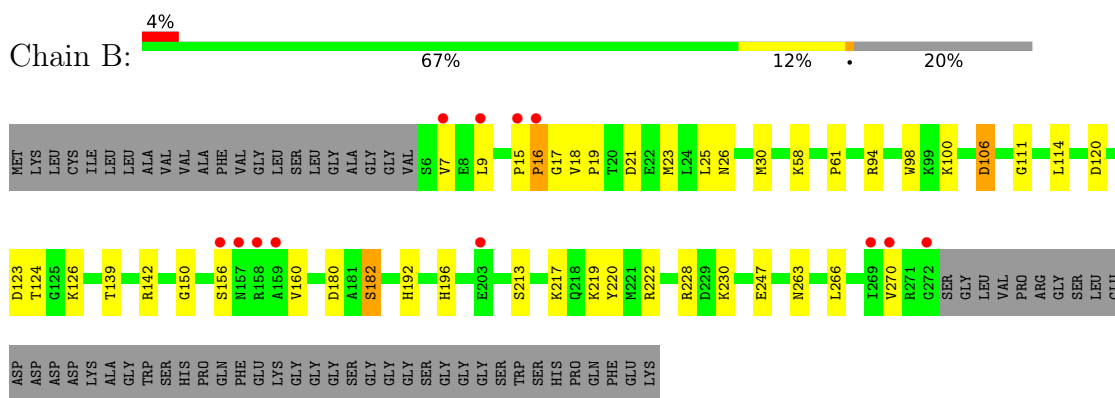
3 Residue-property plots [i](#)

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.

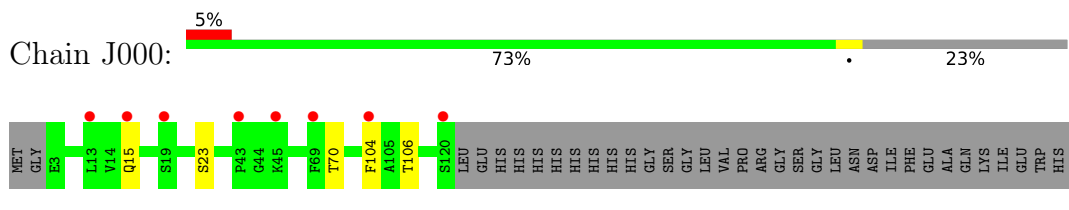
• Molecule 1: Virion membrane protein OPG143



• Molecule 2: Entry-fusion complex protein OPG094



• Molecule 3: VHH D07



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	46.10Å 147.47Å 183.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.09 – 2.50 39.09 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.09-2.50) 99.8 (39.09-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.215 , 0.247 0.222 , 0.253	Depositor DCC
R_{free} test set	2180 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5512	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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	0.33	0/2448	0.87	2/3307 (0.1%)
2	B	0.32	0/2204	0.88	5/2982 (0.2%)
3	J000	0.18	0/912	0.39	0/1234
All	All	0.31	0/5564	0.82	7/7523 (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	B	16	PRO	N-CD-CG	-11.76	85.56	103.20
2	B	16	PRO	N-CA-CB	-9.19	95.13	103.31
2	B	16	PRO	CA-CB-CG	-8.71	87.95	104.50
2	B	142	ARG	CB-CG-CD	6.29	125.76	111.30
1	A	45	THR	N-CA-C	-5.63	99.72	108.90
2	B	17	GLY	N-CA-C	-5.41	104.18	111.54
1	A	240	LYS	N-CA-C	-5.30	101.34	109.76

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	2379	0	2248	66	0
2	B	2153	0	2075	25	0
3	J000	897	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	23	0	0	0	0
4	B	57	0	0	1	0
4	J000	3	0	0	0	0
All	All	5512	0	4323	85	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 10.

All (85) 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:A:81:GLN:HG2	1:A:132:LYS:HE2	1.57	0.87
1:A:55:ILE:HG13	1:A:130:PHE:HB2	1.55	0.84
1:A:68:ASP:HA	2:B:23:MET:HE1	1.60	0.83
1:A:163:TYR:O	1:A:193:ARG:NH2	2.15	0.79
1:A:112:ILE:HG23	1:A:122:ILE:HD11	1.63	0.79
1:A:30:TYR:CD2	1:A:31:PRO:HD3	2.21	0.76
1:A:62:ILE:HG22	1:A:65:MET:HB2	1.73	0.69
2:B:19:PRO:HA	2:B:23:MET:HE2	1.74	0.68
1:A:30:TYR:HD2	1:A:31:PRO:HD3	1.58	0.67
1:A:194:LYS:NZ	2:B:123:ASP:OD1	2.26	0.66
1:A:8:ASN:HA	2:B:7:VAL:HG11	1.78	0.65
1:A:6:THR:OG1	1:A:29:ASN:ND2	2.31	0.64
1:A:12:ILE:HD12	1:A:24:MET:HE1	1.80	0.63
1:A:62:ILE:HD11	1:A:123:ALA:HB1	1.81	0.63
2:B:16:PRO:O	2:B:16:PRO:HG2	1.99	0.62
1:A:35:ARG:HD3	1:A:106:GLU:HB3	1.83	0.61
1:A:35:ARG:HG3	1:A:111:TYR:CE2	2.36	0.61
1:A:111:TYR:HE1	1:A:115:LEU:HD12	1.65	0.61
1:A:13:ALA:HB3	1:A:23:TYR:HB2	1.84	0.60
2:B:19:PRO:HA	2:B:23:MET:CE	2.32	0.60
2:B:180:ASP:OD1	2:B:182:SER:OG	2.20	0.60
2:B:150:GLY:HA2	2:B:192:HIS:CD2	2.37	0.60
1:A:115:LEU:HD23	1:A:119:THR:OG1	2.04	0.58
2:B:120:ASP:O	2:B:124:THR:HG23	2.03	0.58
2:B:124:THR:OG1	2:B:126:LYS:HG3	2.03	0.58
2:B:94:ARG:NH1	2:B:106:ASP:OD2	2.32	0.58
1:A:113:LYS:HD3	1:A:116:LYS:HE3	1.87	0.56
2:B:196:HIS:HE1	4:B:415:HOH:O	1.86	0.56
1:A:16:ILE:HD12	1:A:17:ALA:N	2.20	0.56
1:A:217:ILE:HD13	1:A:220:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:OD2	1:A:140:SER:N	2.40	0.55
2:B:213:SER:O	2:B:217:LYS:HG3	2.06	0.54
1:A:115:LEU:O	1:A:119:THR:OG1	2.26	0.54
1:A:42:GLU:HG2	1:A:58:LYS:N	2.23	0.53
1:A:257:ASP:HA	1:A:260:LEU:HG	1.92	0.52
1:A:49:GLU:HA	1:A:55:ILE:CG2	2.39	0.52
1:A:71:SER:OG	2:B:18:VAL:O	2.24	0.51
1:A:215:GLU:HA	1:A:218:ARG:NH1	2.26	0.51
1:A:30:TYR:HB3	1:A:31:PRO:CD	2.41	0.51
2:B:222:ARG:HD2	2:B:247:GLU:OE1	2.10	0.50
1:A:161:ASN:O	1:A:164:LYS:HE3	2.11	0.49
1:A:113:LYS:O	1:A:116:LYS:HG3	2.12	0.49
2:B:26:ASN:O	2:B:30:MET:HG3	2.12	0.49
1:A:68:ASP:OD2	1:A:68:ASP:N	2.44	0.48
1:A:116:LYS:HB3	1:A:122:ILE:HG23	1.94	0.48
1:A:35:ARG:HG3	1:A:111:TYR:HE2	1.76	0.48
1:A:85:ILE:HD13	1:A:131:ILE:HD13	1.96	0.48
1:A:62:ILE:H	1:A:65:MET:HE3	1.78	0.48
1:A:190:ARG:NH1	1:A:215:GLU:OE2	2.47	0.48
1:A:30:TYR:HB3	1:A:31:PRO:HD2	1.94	0.48
1:A:243:ARG:NH1	1:A:269:GLU:OE1	2.46	0.48
2:B:21:ASP:O	2:B:25:LEU:HG	2.15	0.47
2:B:263:ASN:HA	2:B:266:LEU:HD12	1.96	0.47
1:A:80:LYS:HG2	2:B:21:ASP:OD2	2.14	0.47
1:A:92:SER:OG	1:A:99:SER:O	2.28	0.46
1:A:111:TYR:CE1	1:A:115:LEU:HD12	2.49	0.46
1:A:37:VAL:HG23	1:A:107:VAL:HG13	1.96	0.46
1:A:116:LYS:HD2	1:A:117:HIS:N	2.31	0.46
2:B:219:LYS:HD3	2:B:220:TYR:CZ	2.51	0.46
1:A:132:LYS:O	1:A:133:LYS:HD3	2.16	0.45
1:A:244:ASN:HB3	1:A:279:TRP:CE2	2.52	0.45
1:A:10:ILE:HD12	1:A:10:ILE:HA	1.85	0.45
1:A:94:LYS:NZ	1:A:120:ASP:OD2	2.50	0.45
2:B:100:LYS:HE3	2:B:111:GLY:HA3	1.98	0.45
1:A:29:ASN:OD1	1:A:30:TYR:HB2	2.18	0.44
1:A:169:ASP:O	1:A:173:THR:HG23	2.18	0.44
1:A:34:ASN:O	1:A:35:ARG:HG2	2.18	0.44
1:A:112:ILE:HG23	1:A:122:ILE:CD1	2.43	0.43
1:A:177:ARG:NH2	1:A:202:ASP:OD2	2.51	0.43
2:B:98:TRP:CZ3	2:B:114:LEU:HB2	2.54	0.43
1:A:62:ILE:HD12	1:A:62:ILE:HA	1.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:VAL:HG23	1:A:107:VAL:CG1	2.48	0.43
1:A:26:LEU:HD11	1:A:35:ARG:H	1.84	0.43
1:A:250:TYR:HA	1:A:251:PRO:HD3	1.74	0.42
1:A:73:PHE:CE1	2:B:15:PRO:HG2	2.55	0.42
1:A:240:LYS:HG3	1:A:249:ASN:HD21	1.84	0.42
1:A:188:TRP:CH2	1:A:196:ALA:HA	2.55	0.42
1:A:288:ARG:C	1:A:290:ARG:H	2.27	0.42
1:A:42:GLU:HG2	1:A:58:LYS:H	1.84	0.41
2:B:228:ARG:H	2:B:228:ARG:HG2	1.53	0.41
1:A:26:LEU:HD11	1:A:35:ARG:N	2.36	0.41
1:A:104:GLN:H	1:A:107:VAL:HB	1.86	0.41
2:B:58:LYS:O	2:B:61:PRO:HD3	2.21	0.41
1:A:39:PHE:HA	1:A:100:LEU:O	2.20	0.40
1:A:276:ASP:HB3	1:A:278:LYS:HG2	2.02	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	A	287/358 (80%)	267 (93%)	17 (6%)	3 (1%)	13	25
2	B	265/334 (79%)	253 (96%)	11 (4%)	1 (0%)	30	49
3	J000	116/154 (75%)	111 (96%)	5 (4%)	0	100	100
All	All	668/846 (79%)	631 (94%)	33 (5%)	4 (1%)	22	39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	TYR
1	A	42	GLU
2	B	156	SER

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Mol	Chain	Res	Type
1	A	289	THR

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	A	262/310 (84%)	245 (94%)	17 (6%)	14	29
2	B	239/286 (84%)	232 (97%)	7 (3%)	37	64
3	J000	95/125 (76%)	90 (95%)	5 (5%)	19	38
All	All	596/721 (83%)	567 (95%)	29 (5%)	21	42

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	12	ILE
1	A	26	LEU
1	A	42	GLU
1	A	51	SER
1	A	81	GLN
1	A	85	ILE
1	A	92	SER
1	A	137	LEU
1	A	142	SER
1	A	152	THR
1	A	226	THR
1	A	237	ASN
1	A	267	LEU
1	A	275	ARG
1	A	289	THR
1	A	294	VAL
2	B	9	LEU
2	B	106	ASP
2	B	139	THR
2	B	160	VAL

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Mol	Chain	Res	Type
2	B	182	SER
2	B	230	LYS
2	B	270	VAL
3	J000	15	GLN
3	J000	23	SER
3	J000	70	THR
3	J000	104	PHE
3	J000	106	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	151	ASN
1	A	242	ASN
1	A	244	ASN
1	A	249	ASN
2	B	163	GLN
2	B	191	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	289/358 (80%)	0.75	32 (11%)	12 11	46, 75, 158, 202	0
2	B	267/334 (79%)	0.36	12 (4%)	39 36	46, 66, 123, 165	0
3	J000	118/154 (76%)	0.48	8 (6%)	25 23	68, 86, 121, 145	0
All	All	674/846 (79%)	0.55	52 (7%)	21 20	46, 73, 145, 202	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	269	ILE	5.1
2	B	159	ALA	4.9
1	A	294	VAL	4.7
1	A	16	ILE	4.6
2	B	156	SER	4.4
1	A	34	ASN	4.2
2	B	16	PRO	4.2
1	A	6	THR	4.0
1	A	121	TYR	3.9
1	A	17	ALA	3.8
1	A	10	ILE	3.7
1	A	118	ALA	3.6
3	J000	43	PRO	3.3
1	A	88	GLU	3.1
2	B	272	GLY	3.1
2	B	270	VAL	3.0
3	J000	15	GLN	3.0
1	A	107	VAL	3.0
3	J000	19	SER	3.0
2	B	15	PRO	3.0
1	A	33	TYR	3.0
1	A	19	ILE	3.0
1	A	120	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	9	ARG	2.9
2	B	158	ARG	2.8
1	A	7	LEU	2.8
1	A	12	ILE	2.8
1	A	36	ALA	2.8
1	A	95	PHE	2.6
3	J000	104	PHE	2.5
3	J000	120	SER	2.5
2	B	7	VAL	2.5
1	A	153	LYS	2.5
1	A	138	GLY	2.4
2	B	9	LEU	2.4
1	A	30	TYR	2.4
2	B	157	ASN	2.3
1	A	11	LYS	2.3
1	A	35	ARG	2.3
1	A	123	ALA	2.3
1	A	28	PHE	2.2
3	J000	45	LYS	2.2
1	A	130	PHE	2.2
1	A	91	SER	2.2
1	A	55	ILE	2.1
1	A	261	GLY	2.1
2	B	203	GLU	2.1
3	J000	13	LEU	2.0
1	A	122	ILE	2.0
1	A	105	ASN	2.0
1	A	139	ASP	2.0
3	J000	69	PHE	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.