



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2024 – 08:48 AM JST

PDB ID : 5ZL2  
Title : Crystal structure of Bourbon virus envelope glycoprotein at pH8.0  
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Deposited on : 2018-03-26  
Resolution : 2.70 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](mailto: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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

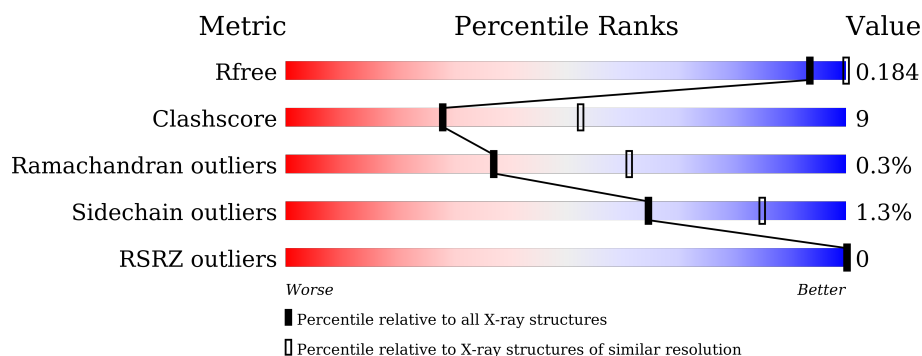
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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  $\geq 3$ , 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	467	 69% 14% 17%
1	B	467	 63% 19% 17%
1	C	467	 65% 18% 17%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9383 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 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3089	1960	528	580	21			
1	B	388	Total	C	N	O	S	0	0	0
			3089	1960	528	580	21			
1	C	388	Total	C	N	O	S	0	0	0
			3089	1960	528	580	21			

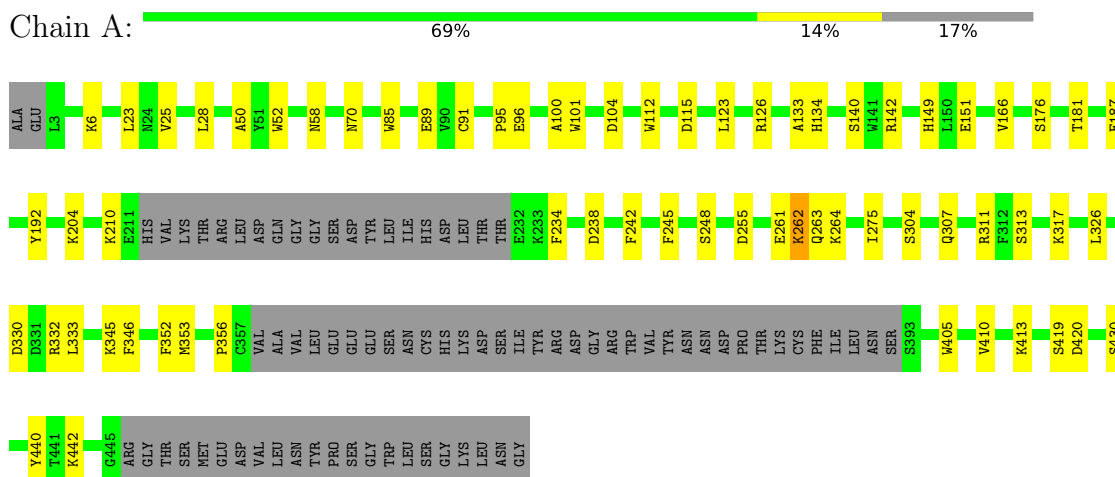
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	47	Total	O	0	0
			47	47		
2	C	38	Total	O	0	0
			38	38		

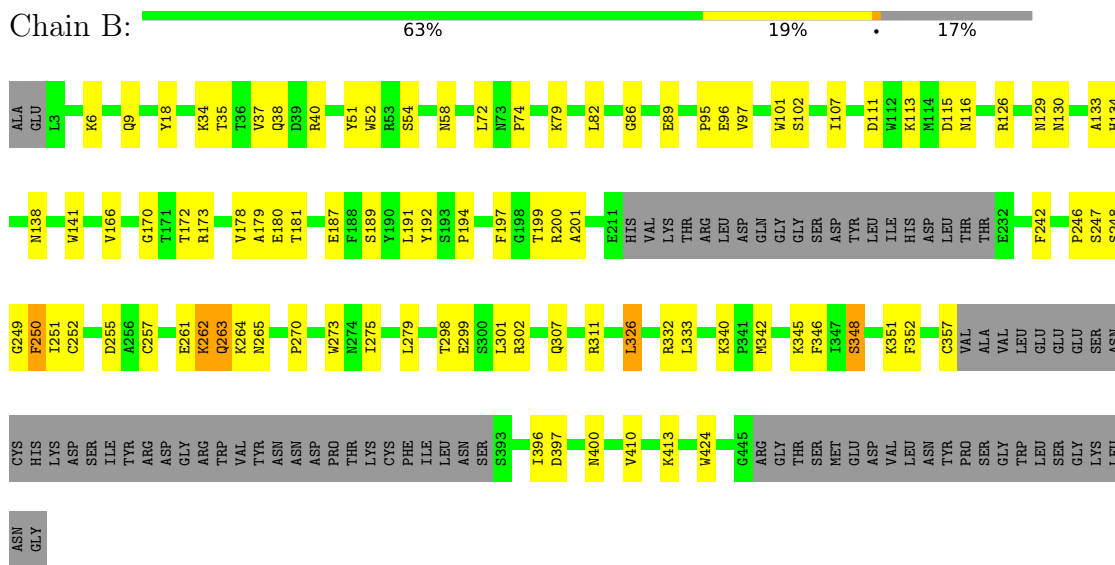
### 3 Residue-property plots

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: Envelope glycoprotein



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ALA	GLU	L3	C4	N5	K6	Q7	Q8	G11	P12	S21	V25	S26	R27	I30	V37	R40	F44	Y51	S54	N73	P74	K75	K79	D80	E81	L82	K83	T84	W85	V90	P95	E96	V97	W101	W112	N116	K117	K121	E122	L123	R126											
A133	H134			N138	L139	S140	W141	V145	A156	T159	A163		M177	V178	F182	Y190	V196	F197	K204	P207	C208	F209	K210	E211	HIS	VAL	LYS	THR	ARG	LEU	ASP	GLN	GLY	SER	ASP	TYR	LEU	ILE	HIS	ASP	LEU	THR	E232	K237	D238	G239	D240					
K241	F242		F250		L253	F254	D255	Y258	K259	N260	E261	K262	Q263	K264		P270	E297	L303	S324	K328	R332		P341	M342	A343		F346		F352	K353	V354	C357	VAL	ALA	VAL	LEU	GLU	GLU	GLU	SER	ASN	CYS	HIS	LYS	ASP	SER	ILE	TYR	ARG	ASP	GLY	ARG
TRP	VAL	TYR	ASN	ASN	ASP	PRO	THR	LYS	CYS	PHE	ILE	LEU	ASN	SER	S393	W405	V410	K413		D422	Y440	T441	K442		G445	ARG	GLY	THR	SER	MET	GLU	ASP	VAL	LEU	ASN	TYR	PRO	SER	GLY	TRP	SER	SER	GLY	LYS	LEU	ASN	GLY					

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.25Å 102.25Å 134.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.79 – 2.70 47.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	80.6 (47.79-2.70) 80.7 (47.79-2.70)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.201 , 0.240 0.159 , 0.184	Depositor DCC
$R_{free}$ test set	1676 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.8	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 21.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.32$ , $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.399 for -h,-k,l 0.417 for h,-h-k,-l 0.427 for -k,-h,-l	Xtriage
Reported twinning fraction	0.480 for -k,-h,-l	Depositor
Outliers	0 of 34756 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9383	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.26	0/3165	0.46	0/4284
1	B	0.27	0/3165	0.46	0/4284
1	C	0.29	0/3165	0.45	0/4284
All	All	0.28	0/9495	0.46	0/12852

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	TRP	Peptide
1	A	262	LYS	Peptide
1	B	101	TRP	Peptide
1	B	262	LYS	Peptide
1	C	101	TRP	Peptide
1	C	262	LYS	Peptide

## 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	3089	0	2996	36	2
1	B	3089	0	2996	67	0
1	C	3089	0	2996	57	0
2	A	31	0	0	4	1
2	B	47	0	0	12	0
2	C	38	0	0	11	0
All	All	9383	0	8988	160	2

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 (160) 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:C:90:VAL:HG11	1:C:117:LYS:HG3	1.68	0.76
1:C:440:TYR:O	1:C:442:LYS:NZ	2.23	0.72
1:A:166:VAL:HG11	1:A:275:ILE:HD11	1.72	0.71
1:B:173:ARG:NH2	2:B:508:HOH:O	2.24	0.71
1:B:37:VAL:HG13	1:B:199:THR:HG23	1.71	0.71
1:B:326:LEU:CD2	1:B:333:LEU:HD22	2.21	0.71
1:B:255:ASP:OD2	1:B:413:LYS:NZ	2.24	0.70
1:B:249:GLY:N	2:B:507:HOH:O	2.23	0.70
1:B:166:VAL:O	2:B:501:HOH:O	2.10	0.69
1:B:130:ASN:OD1	2:B:502:HOH:O	2.11	0.68
1:C:7:GLN:NE2	1:C:8:GLN:OE1	2.27	0.67
1:A:330:ASP:OD1	2:A:501:HOH:O	2.13	0.67
1:C:255:ASP:OD2	1:C:413:LYS:NZ	2.27	0.67
1:A:242:PHE:CZ	1:A:410:VAL:HG13	2.31	0.65
1:B:40:ARG:O	2:B:503:HOH:O	2.14	0.65
1:C:324:SER:O	1:C:328:LYS:NZ	2.30	0.65
1:B:424:TRP:NE1	2:B:501:HOH:O	2.30	0.64
1:C:422:ASP:OD2	2:C:501:HOH:O	2.15	0.63
1:C:346:PHE:HA	1:C:352:PHE:HA	1.79	0.62
1:B:326:LEU:HD22	1:B:333:LEU:HD22	1.81	0.62
1:B:178:VAL:HG23	1:B:179:ALA:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:GLU:OE1	2:C:502:HOH:O	2.16	0.60
1:A:52:TRP:CH2	1:A:70:ASN:HB3	2.37	0.60
1:C:261:GLU:HA	1:C:264:LYS:HB2	1.84	0.59
1:A:326:LEU:HD23	1:A:333:LEU:HD22	1.84	0.59
1:B:180:GLU:HB3	1:B:191:LEU:HD11	1.85	0.59
1:A:133:ALA:O	1:A:134:HIS:ND1	2.35	0.59
1:A:420:ASP:O	2:A:502:HOH:O	2.16	0.58
1:A:58:ASN:O	1:A:133:ALA:N	2.36	0.58
1:C:90:VAL:CG1	1:C:117:LYS:HG3	2.33	0.58
1:A:23:LEU:HD23	1:A:25:VAL:H	1.69	0.58
1:B:54:SER:O	2:B:504:HOH:O	2.17	0.58
1:C:242:PHE:CZ	1:C:410:VAL:HG13	2.38	0.57
1:A:204:LYS:NZ	1:A:238:ASP:OD1	2.26	0.57
1:C:332:ARG:HH22	1:C:341:PRO:HA	1.69	0.57
1:B:326:LEU:HD23	1:B:333:LEU:HD22	1.87	0.56
1:B:129:ASN:ND2	2:B:509:HOH:O	2.38	0.56
1:C:96:GLU:OE2	1:C:126:ARG:NH2	2.37	0.55
1:A:346:PHE:HA	1:A:352:PHE:HA	1.88	0.55
1:C:25:VAL:HA	1:C:210:LYS:O	2.06	0.55
1:B:181:THR:HG23	1:B:192:TYR:HB3	1.87	0.55
1:B:178:VAL:HG23	1:B:179:ALA:N	2.22	0.55
1:B:6:LYS:O	1:B:9:GLN:NE2	2.40	0.55
1:B:332:ARG:NH2	1:B:357:CYS:SG	2.75	0.54
1:B:242:PHE:CZ	1:B:410:VAL:HG13	2.43	0.53
1:B:299:GLU:HA	1:B:302:ARG:HD3	1.89	0.53
1:A:85:TRP:O	1:A:89:GLU:N	2.41	0.53
1:A:345:LYS:O	1:A:353:MET:N	2.40	0.53
1:B:273:TRP:CZ3	1:B:275:ILE:HA	2.43	0.53
1:C:159:THR:O	2:C:503:HOH:O	2.19	0.53
1:C:405:TRP:NE1	2:C:509:HOH:O	2.33	0.52
1:C:121:LYS:NZ	1:C:141:TRP:O	2.43	0.51
1:A:115:ASP:N	1:A:115:ASP:OD1	2.43	0.51
1:B:250:PHE:CD2	1:B:270:PRO:HB3	2.47	0.50
1:B:250:PHE:CG	1:B:270:PRO:HB3	2.46	0.50
1:A:181:THR:HG23	1:A:192:TYR:HB3	1.93	0.50
1:B:52:TRP:HE3	1:B:72:LEU:HG	1.76	0.50
1:A:440:TYR:CZ	1:A:442:LYS:HE3	2.46	0.49
1:B:58:ASN:O	1:B:133:ALA:N	2.45	0.49
1:B:35:THR:HG22	1:B:199:THR:HG21	1.94	0.48
1:B:246:PRO:HG3	1:B:251:ILE:HB	1.94	0.48
1:C:80:ASP:O	1:C:84:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:VAL:CG1	1:B:199:THR:HG23	2.42	0.48
1:C:332:ARG:HH12	1:C:342:MET:N	2.12	0.48
1:A:50:ALA:HB2	1:A:187:GLU:HG2	1.96	0.48
1:B:74:PRO:HB3	1:B:187:GLU:HG2	1.96	0.48
1:A:149:HIS:NE2	1:A:151:GLU:OE1	2.35	0.48
1:B:346:PHE:HA	1:B:352:PHE:HA	1.94	0.48
1:B:348:SER:HB3	1:B:351:LYS:HG2	1.96	0.48
1:B:199:THR:HG22	1:B:200:ARG:H	1.78	0.47
1:C:156:ALA:O	2:C:503:HOH:O	2.20	0.47
1:A:261:GLU:HA	1:A:264:LYS:HB2	1.97	0.47
1:A:142:ARG:NH1	1:A:187:GLU:OE2	2.46	0.47
1:C:204:LYS:NZ	1:C:238:ASP:OD1	2.43	0.47
1:C:82:LEU:HD23	2:C:514:HOH:O	2.15	0.47
1:B:97:VAL:HG11	1:B:107:ILE:HG21	1.97	0.47
1:C:253:LEU:HD12	1:C:258:TYR:HE1	1.80	0.47
1:A:25:VAL:HA	1:A:210:LYS:O	2.15	0.46
1:A:96:GLU:HG3	1:A:126:ARG:HH22	1.79	0.46
1:C:79:LYS:HG2	1:C:83:LYS:HE3	1.96	0.46
1:C:27:ARG:HH22	1:C:207:PRO:CB	2.28	0.46
1:A:261:GLU:HG3	1:A:264:LYS:HB2	1.98	0.46
1:C:250:PHE:CG	1:C:270:PRO:HB3	2.51	0.46
1:B:34:LYS:O	1:B:201:ALA:HA	2.16	0.46
1:B:95:PRO:HA	1:B:116:ASN:ND2	2.31	0.46
1:C:95:PRO:HA	1:C:116:ASN:ND2	2.31	0.46
1:A:100:ALA:HB1	1:A:104:ASP:HB2	1.98	0.46
1:B:340:LYS:O	1:B:342:MET:HG2	2.16	0.46
1:B:96:GLU:HG3	1:B:126:ARG:HH22	1.81	0.45
1:A:28:LEU:HD23	2:A:510:HOH:O	2.16	0.45
1:C:37:VAL:HG11	1:C:163:ALA:HB2	1.98	0.45
1:A:234:PHE:HB2	1:A:245:PHE:HB3	1.98	0.45
1:A:307:GLN:O	1:A:311:ARG:HG3	2.17	0.45
1:C:262:LYS:O	1:C:263:GLN:HB2	2.16	0.45
1:C:240:ASP:HB2	1:C:413:LYS:HB2	1.98	0.45
1:C:21:SER:O	2:C:504:HOH:O	2.21	0.45
1:C:346:PHE:CG	1:C:352:PHE:HB3	2.52	0.44
1:B:51:TYR:HB3	1:B:141:TRP:CE3	2.53	0.44
1:B:170:GLY:HA2	1:B:279:LEU:HD11	1.99	0.44
1:C:54:SER:HB3	1:C:138:ASN:HB2	1.99	0.44
1:C:133:ALA:O	1:C:134:HIS:ND1	2.50	0.44
1:A:332:ARG:NE	1:A:332:ARG:HA	2.33	0.44
1:B:194:PRO:HG2	1:B:197:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLU:HA	1:B:264:LYS:HB2	1.99	0.44
1:B:397:ASP:OD1	1:B:400:ASN:HA	2.18	0.44
1:C:123:LEU:HB2	1:C:140:SER:HB3	2.00	0.44
1:A:346:PHE:CD1	1:A:352:PHE:HB3	2.52	0.44
1:B:138:ASN:ND2	2:B:504:HOH:O	2.27	0.44
1:C:30:ILE:HD12	1:C:208:CYS:SG	2.58	0.44
1:C:303:LEU:HD23	1:C:303:LEU:HA	1.82	0.44
1:B:18:TYR:OH	1:B:311:ARG:NH2	2.47	0.44
1:B:86:GLY:HA2	2:B:522:HOH:O	2.18	0.44
1:A:123:LEU:HB2	1:A:140:SER:HB3	2.00	0.43
1:B:82:LEU:HD22	1:B:189:SER:HB3	2.00	0.43
1:C:44:PHE:CZ	1:C:190:TYR:HB3	2.54	0.43
1:C:51:TYR:HB3	1:C:141:TRP:CE3	2.53	0.43
1:C:342:MET:SD	1:C:354:VAL:HG21	2.58	0.43
1:B:247:SER:OG	1:B:248:SER:N	2.51	0.43
1:C:51:TYR:CZ	1:C:73:ASN:HB2	2.53	0.43
1:C:97:VAL:HB	1:C:139:LEU:HB3	2.00	0.43
1:B:262:LYS:O	1:B:263:GLN:HB2	2.18	0.43
1:B:79:LYS:HZ3	1:B:191:LEU:HD13	1.84	0.43
1:C:11:GLY:HA3	1:C:12:PRO:HA	1.90	0.43
1:B:89:GLU:HA	2:B:522:HOH:O	2.17	0.43
1:C:134:HIS:N	2:C:511:HOH:O	2.52	0.43
1:C:346:PHE:CD1	1:C:352:PHE:HB3	2.54	0.43
1:A:419:SER:N	2:A:514:HOH:O	2.52	0.42
1:B:248:SER:O	1:B:263:GLN:HG2	2.20	0.42
1:B:38:GLN:O	1:B:200:ARG:NH2	2.52	0.42
1:B:346:PHE:CG	1:B:352:PHE:HB3	2.54	0.42
1:A:176:SER:H	1:A:181:THR:HB	1.84	0.42
1:C:177:MET:SD	1:C:178:VAL:HG13	2.60	0.42
1:B:111:ASP:O	1:B:113:LYS:HG2	2.19	0.42
1:B:252:CYS:O	1:B:273:TRP:HD1	2.02	0.42
1:C:343:ALA:N	2:C:507:HOH:O	2.52	0.42
1:C:182:PHE:HD1	2:C:514:HOH:O	2.03	0.42
1:C:250:PHE:CD2	1:C:270:PRO:HB3	2.54	0.42
1:B:35:THR:HB	1:B:257:CYS:HB2	2.01	0.42
1:B:396:ILE:HD12	1:B:396:ILE:HA	1.76	0.42
1:C:6:LYS:HB3	1:C:6:LYS:HE3	1.84	0.42
1:C:75:LYS:HD3	1:C:75:LYS:HA	1.87	0.42
1:A:255:ASP:OD2	1:A:413:LYS:NZ	2.53	0.41
1:C:95:PRO:HD3	1:C:112:TRP:HB3	2.02	0.41
1:C:177:MET:H	1:C:177:MET:HG3	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:SER:O	1:A:317:LYS:HG3	2.21	0.41
1:C:85:TRP:HB3	1:C:145:VAL:HG21	2.02	0.41
1:B:248:SER:N	2:B:507:HOH:O	2.54	0.41
1:C:197:PHE:N	1:C:197:PHE:CD1	2.89	0.41
1:B:298:THR:O	1:B:301:LEU:HB3	2.20	0.41
1:B:97:VAL:HG21	1:B:107:ILE:HD13	2.01	0.41
1:B:102:SER:HB3	1:B:134:HIS:CG	2.56	0.41
1:B:348:SER:HB3	1:B:351:LYS:CG	2.51	0.41
1:A:261:GLU:O	1:A:262:LYS:HB2	2.21	0.40
1:B:115:ASP:OD1	1:B:115:ASP:N	2.54	0.40
1:B:166:VAL:HG12	1:B:172:THR:HG22	2.03	0.40
1:B:178:VAL:CG2	1:B:179:ALA:H	2.33	0.40
1:C:4:CYS:O	2:C:505:HOH:O	2.22	0.40
1:C:196:VAL:C	1:C:197:PHE:HD1	2.25	0.40
1:A:95:PRO:HD3	1:A:112:TRP:HB3	2.03	0.40
1:B:262:LYS:HB2	1:B:262:LYS:HE3	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:SER:OG	1:A:405:TRP:O[2_555]	2.15	0.05
1:A:356:PRO:O	2:A:512:HOH:O[2_555]	2.19	0.01

## 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	382/467 (82%)	362 (95%)	18 (5%)	2 (0%)	25	49
1	B	382/467 (82%)	362 (95%)	19 (5%)	1 (0%)	37	61
1	C	382/467 (82%)	361 (94%)	20 (5%)	1 (0%)	37	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1146/1401 (82%)	1085 (95%)	57 (5%)	4 (0%)	37 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	263	GLN
1	C	263	GLN
1	A	6	LYS
1	A	263	GLN

### 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	344/414 (83%)	341 (99%)	3 (1%)	75 90
1	B	344/414 (83%)	338 (98%)	6 (2%)	56 81
1	C	344/414 (83%)	340 (99%)	4 (1%)	67 86
All	All	1032/1242 (83%)	1019 (99%)	13 (1%)	65 85

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	CYS
1	A	248	SER
1	A	430	SER
1	B	250	PHE
1	B	265	ASN
1	B	307	GLN
1	B	326	LEU
1	B	345	LYS
1	B	348	SER
1	C	40	ARG
1	C	204	LYS
1	C	237	LYS

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Mol	Chain	Res	Type
1	C	259	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	128	ASN
1	B	241	ASN
1	B	265	ASN
1	C	7	GLN

### 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	388/467 (83%)	-1.85	0 100 100	8, 32, 68, 146	0
1	B	388/467 (83%)	-1.72	0 100 100	10, 40, 108, 188	0
1	C	388/467 (83%)	-1.66	0 100 100	12, 48, 117, 194	0
All	All	1164/1401 (83%)	-1.74	0 100 100	8, 39, 106, 194	0

There are no RSRZ outliers to report.

### 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.