



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2023 – 02:36 PM EDT

PDB ID : 2WZR  
Title : The Structure of Foot and Mouth Disease Virus Serotype SAT1  
Authors : Adams, P.; Lea, S.; Newman, J.; Blakemore, W.; King, A.; Stuart, D.; Fry, E.  
Deposited on : 2009-12-02  
Resolution : 3.00 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 : 2.35.1  
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) : 2.35.1

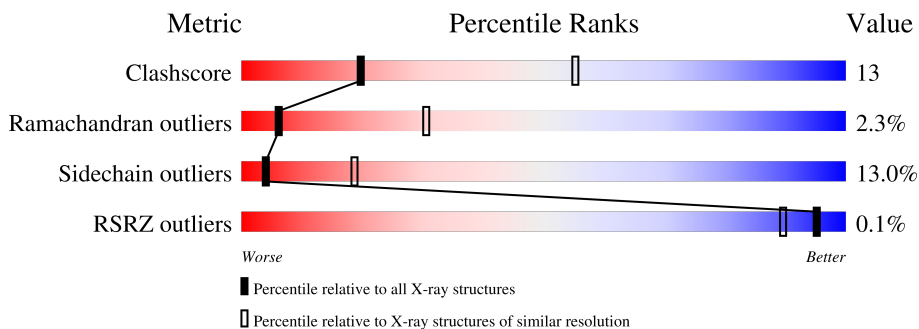
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	1	219	
2	2	219	
3	3	221	
4	4	85	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5210 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 POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	194	1501	947	266	283	5	0	0	2

- Molecule 2 is a protein called POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	207	1639	1041	282	312	4	0	0	0

- Molecule 3 is a protein called POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	221	1717	1099	276	333	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	163	PHE	ILE	conflict	UNP Q6PMU1

- Molecule 4 is a protein called POLYPROTEIN.

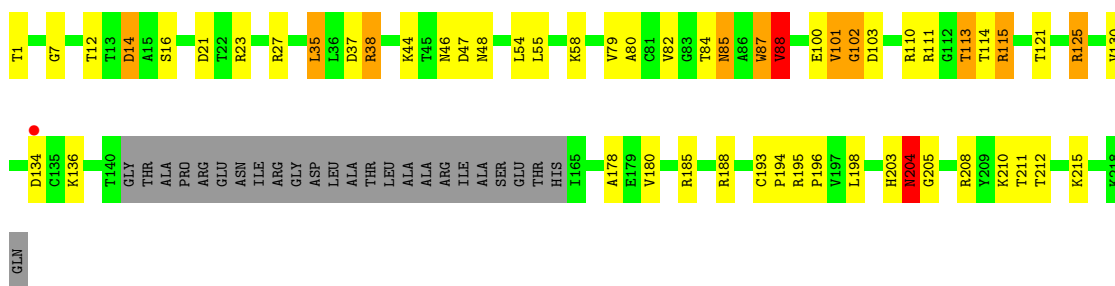
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	47	353	220	59	72	2	0	0	1

### 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.

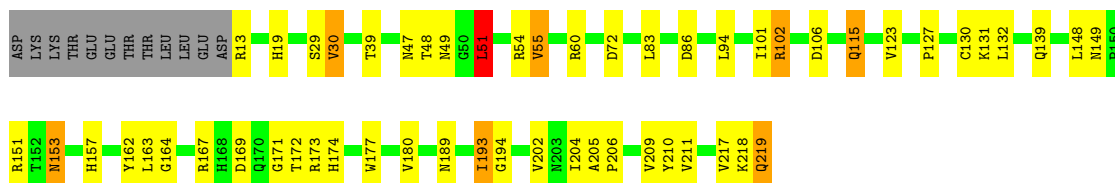
#### • Molecule 1: POLYPROTEIN

Chain 1: 



#### • Molecule 2: POLYPROTEIN

Chain 2: 



#### • Molecule 3: POLYPROTEIN

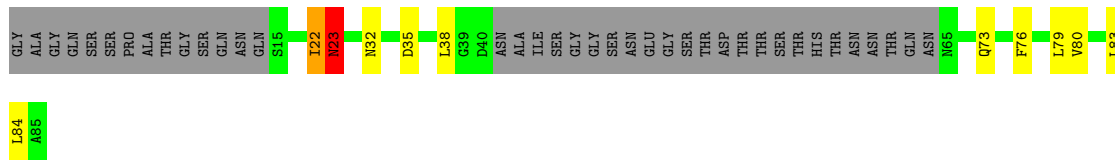
Chain 3: 



#### • Molecule 4: POLYPROTEIN

Chain 4: 





L84  
R65

## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	305.14Å 305.14Å 723.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	17.00 – 3.00 16.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	60.1 (17.00-3.00) 58.7 (16.99-3.00)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.27 (at 3.02Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.230 , (Not available) 0.359 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.25$ , $\langle L^2 \rangle = 0.09$	Xtriage
Estimated twinning fraction	0.247 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l 0.246 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/ 3*k+1/3*l 0.248 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+ 1/3*l,-4/3*h+4/3*k+1/3*l 0.248 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3* k-1/3*l 0.248 for -1/3*h-2/3*k+1/3*l,-2/3*h-1/3*k- 1/3*l,4/3*h-4/3*k-1/3*l 0.247 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3 *k-1/3*l 0.329 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.49	EDS
Total number of atoms	5210	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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 [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	1	0.64	0/1536	0.99	4/2097 (0.2%)
2	2	0.63	0/1680	0.88	1/2293 (0.0%)
3	3	0.68	1/1774 (0.1%)	0.98	3/2427 (0.1%)
4	4	0.69	0/358	0.80	0/481
All	All	0.66	1/5348 (0.0%)	0.94	8/7298 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	163	PHE	CB-CG	-6.08	1.41	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	87	TRP	N-CA-C	8.27	133.33	111.00
3	3	220	ARG	N-CA-C	7.47	131.16	111.00
3	3	198	GLY	N-CA-C	-6.12	97.80	113.10
1	1	14	ASP	CB-CA-C	-5.74	98.93	110.40
2	2	51	LEU	CA-CB-CG	5.66	128.32	115.30
1	1	198	LEU	CA-CB-CG	5.56	128.09	115.30
1	1	88	VAL	CB-CA-C	-5.11	101.70	111.40
3	3	219	SER	N-CA-C	5.09	124.76	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	1	1501	0	1482	36	0
2	2	1639	0	1601	41	0
3	3	1717	0	1601	67	0
4	4	353	0	327	7	0
All	All	5210	0	5011	129	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 13.

All (129) 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)
1:1:100:GLU:HB2	3:3:220:ARG:HH22	1.26	1.00
1:1:100:GLU:HB2	3:3:220:ARG:NH2	1.92	0.83
3:3:108:HIS:HB2	3:3:203:THR:HG22	1.62	0.82
2:2:172:THR:HG22	2:2:173:ARG:H	1.46	0.81
1:1:35:LEU:O	1:1:38:ARG:HD2	1.80	0.80
3:3:131:HIS:HB3	3:3:132:PRO:HD3	1.65	0.78
3:3:83:HIS:HD2	3:3:85:ASN:H	1.30	0.77
2:2:219:GLN:NE2	3:3:132:PRO:HG2	2.03	0.73
3:3:43:ASN:HD22	3:3:45:LEU:H	1.38	0.71
2:2:49:ASN:HD22	3:3:162:TYR:H	1.37	0.71
1:1:100:GLU:CB	3:3:220:ARG:HH22	2.04	0.70
3:3:83:HIS:CD2	3:3:85:ASN:H	2.11	0.69
2:2:51:LEU:HD23	3:3:163:PHE:CZ	2.29	0.68
3:3:63:VAL:CG1	3:3:74:LEU:HB3	2.24	0.68
3:3:64:GLN:CG	3:3:197:ASP:HB3	2.25	0.67
1:1:211:THR:HG22	1:1:212:THR:H	1.59	0.66
3:3:100:GLN:NE2	3:3:213:ARG:HH11	1.96	0.64
1:1:121:THR:HG22	3:3:214:MET:HE1	1.79	0.64
1:1:102:GLY:O	1:1:103:ASP:HB2	1.97	0.64
2:2:115:GLN:HE21	2:2:115:GLN:H	1.44	0.64
2:2:131:LYS:HG2	2:2:132:LEU:N	2.11	0.64
1:1:110:ARG:NE	1:1:110:ARG:HA	2.13	0.63
3:3:112:THR:HB	3:3:199:ALA:O	1.99	0.63
3:3:52:PRO:HB3	3:3:203:THR:HG23	1.80	0.63
3:3:63:VAL:HG13	3:3:74:LEU:HB3	1.80	0.63
3:3:104:THR:CG2	3:3:207:GLY:HA3	2.29	0.62
1:1:125:ARG:NH2	2:2:164:GLY:O	2.33	0.61
2:2:115:GLN:H	2:2:115:GLN:NE2	1.97	0.61
1:1:82:VAL:HG22	1:1:113:THR:HB	1.82	0.61
2:2:106:ASP:OD2	2:2:157:HIS:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:54:ARG:HG3	2:2:55:VAL:N	2.15	0.61
1:1:85:ASN:HB2	1:1:178:ALA:HB3	1.83	0.60
2:2:19:HIS:HE1	2:2:106:ASP:OD1	1.84	0.60
3:3:193:THR:HG22	3:3:193:THR:O	2.03	0.58
4:4:22:ILE:HG22	4:4:23:ASN:ND2	2.19	0.58
2:2:153:ASN:HD22	2:2:153:ASN:N	2.01	0.58
2:2:49:ASN:HB3	2:2:51:LEU:HD22	1.86	0.57
2:2:172:THR:HG22	2:2:173:ARG:N	2.18	0.57
1:1:80:ALA:HA	1:1:114:THR:O	2.04	0.57
3:3:161:PRO:HB2	3:3:163:PHE:HE1	1.70	0.57
3:3:220:ARG:HB2	3:3:221:GLN:OE1	2.04	0.56
4:4:22:ILE:O	4:4:23:ASN:HB3	2.04	0.56
2:2:167:ARG:NH2	3:3:167:ASP:OD1	2.40	0.55
3:3:100:GLN:HE22	3:3:213:ARG:HH11	1.54	0.55
3:3:100:GLN:HE22	3:3:213:ARG:NH1	2.05	0.55
3:3:131:HIS:CB	3:3:132:PRO:HD3	2.36	0.54
2:2:172:THR:O	2:2:173:ARG:HB2	2.08	0.53
2:2:219:GLN:CD	3:3:132:PRO:HG2	2.28	0.53
3:3:63:VAL:HG11	3:3:74:LEU:HB3	1.91	0.53
3:3:104:THR:HG23	3:3:207:GLY:HA3	1.90	0.53
3:3:131:HIS:O	3:3:132:PRO:C	2.46	0.53
1:1:100:GLU:HB3	3:3:220:ARG:HH12	1.74	0.52
3:3:43:ASN:ND2	3:3:45:LEU:H	2.03	0.52
3:3:64:GLN:NE2	3:3:197:ASP:HB3	2.24	0.52
2:2:101:ILE:HG13	2:2:211:VAL:HG12	1.92	0.52
3:3:66:GLN:HG3	3:3:67:SER:N	2.24	0.52
3:3:103:GLY:HA3	3:3:210:PHE:HA	1.92	0.52
1:1:79:VAL:O	1:1:115:ARG:HA	2.10	0.51
2:2:202:VAL:CG1	2:2:204:ILE:HG13	2.40	0.51
2:2:47:ASN:O	3:3:163:PHE:HA	2.10	0.51
2:2:217:VAL:O	2:2:218:LYS:HB2	2.11	0.51
3:3:64:GLN:CD	3:3:197:ASP:HB3	2.31	0.51
2:2:131:LYS:HG2	2:2:132:LEU:H	1.76	0.51
2:2:163:LEU:HD22	2:2:177:TRP:CZ2	2.46	0.51
3:3:131:HIS:HB3	3:3:132:PRO:CD	2.40	0.51
3:3:163:PHE:N	3:3:163:PHE:CD1	2.79	0.50
2:2:55:VAL:HG21	2:2:94:LEU:HD11	1.93	0.50
3:3:45:LEU:HA	3:3:48:ALA:HB3	1.94	0.50
1:1:37:ASP:OD2	1:1:185:ARG:HD2	2.12	0.49
1:1:211:THR:HG22	1:1:212:THR:N	2.27	0.49
3:3:65:THR:OG1	3:3:197:ASP:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:193:THR:O	3:3:193:THR:CG2	2.60	0.48
2:2:202:VAL:HG12	2:2:204:ILE:HG13	1.95	0.48
1:1:100:GLU:HB3	3:3:220:ARG:NH1	2.28	0.48
3:3:64:GLN:NE2	3:3:197:ASP:CB	2.76	0.48
3:3:84:LYS:O	3:3:87:LYS:HB3	2.14	0.48
3:3:163:PHE:N	3:3:163:PHE:HD1	2.12	0.47
1:1:188:ARG:NH1	4:4:35:ASP:OD1	2.48	0.47
3:3:104:THR:HG22	3:3:207:GLY:HA3	1.95	0.47
2:2:54:ARG:HB2	2:2:210:TYR:CE2	2.50	0.47
3:3:193:THR:O	3:3:194:HIS:CB	2.62	0.46
2:2:102:ARG:HD3	2:2:102:ARG:C	2.36	0.46
1:1:101:VAL:O	1:1:102:GLY:C	2.55	0.46
1:1:203:HIS:O	1:1:204:ASN:HB2	2.16	0.46
1:1:111:ARG:HD3	3:3:9:ASP:OD2	2.17	0.45
3:3:131:HIS:CB	3:3:132:PRO:CD	2.95	0.45
3:3:43:ASN:HD22	3:3:45:LEU:N	2.08	0.45
3:3:118:LYS:H	3:3:193:THR:CG2	2.30	0.44
1:1:204:ASN:HB3	1:1:205:GLY:H	1.59	0.44
4:4:79:LEU:CD2	4:4:83:LEU:HB2	2.48	0.44
3:3:45:LEU:HA	3:3:45:LEU:HD23	1.78	0.43
1:1:196:PRO:HB3	2:2:139:GLN:HB2	1.99	0.43
3:3:52:PRO:HG3	3:3:205:SER:HB3	2.00	0.43
3:3:64:GLN:HG3	3:3:197:ASP:HB3	2.00	0.43
1:1:47:ASP:O	1:1:48:ASN:HB2	2.19	0.43
2:2:153:ASN:HD22	2:2:153:ASN:H	1.66	0.43
1:1:14:ASP:HB2	1:1:16:SER:OG	2.19	0.43
3:3:193:THR:O	3:3:194:HIS:HB2	2.19	0.43
2:2:13:ARG:HD2	2:2:29:SER:O	2.19	0.43
3:3:78:ASP:OD1	3:3:180:SER:HB2	2.18	0.43
3:3:131:HIS:O	3:3:133:LEU:N	2.52	0.43
2:2:193:ILE:HD12	2:2:193:ILE:HG23	1.69	0.42
2:2:102:ARG:NH1	2:2:162:TYR:HB3	2.34	0.42
1:1:100:GLU:CB	3:3:220:ARG:NH2	2.70	0.42
2:2:205:ALA:HA	2:2:206:PRO:HD3	1.87	0.42
3:3:79:LEU:HD12	3:3:125:TYR:HE1	1.84	0.42
1:1:55:LEU:HD23	1:1:55:LEU:HA	1.86	0.42
3:3:168:TYR:CD1	3:3:213:ARG:HD2	2.55	0.42
1:1:195:ARG:NH2	2:2:127:PRO:O	2.53	0.42
4:4:23:ASN:N	4:4:23:ASN:HD22	2.17	0.42
1:1:54:LEU:HA	1:1:54:LEU:HD23	1.72	0.41
1:1:35:LEU:O	1:1:38:ARG:CD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:49:ASN:ND2	3:3:162:TYR:H	2.13	0.41
2:2:189:ASN:ND2	2:2:194:GLY:HA3	2.35	0.41
2:2:204:ILE:HG22	2:2:205:ALA:N	2.36	0.41
3:3:112:THR:O	3:3:112:THR:HG23	2.20	0.41
2:2:55:VAL:O	2:2:55:VAL:HG22	2.20	0.41
2:2:148:LEU:HD23	2:2:148:LEU:HA	1.92	0.41
3:3:161:PRO:HB2	3:3:163:PHE:CE1	2.53	0.41
2:2:172:THR:O	2:2:174:HIS:N	2.51	0.41
3:3:68:ASN:O	3:3:69:SER:HB3	2.21	0.41
4:4:76:PHE:HE2	4:4:80:VAL:HG23	1.85	0.41
1:1:87:TRP:O	1:1:88:VAL:C	2.59	0.41
1:1:121:THR:HG22	3:3:214:MET:CE	2.47	0.41
3:3:35:THR:O	3:3:36:LEU:HB2	2.21	0.41
1:1:7:GLY:HA2	2:2:30:VAL:HG13	2.03	0.40
1:1:193:CYS:HA	1:1:194:PRO:HD2	1.88	0.40
1:1:44:LYS:HA	1:1:180:VAL:O	2.21	0.40
1:1:188:ARG:HD2	4:4:32:ASN:ND2	2.36	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	1	190/219 (87%)	173 (91%)	12 (6%)	5 (3%)	5	27
2	2	205/219 (94%)	192 (94%)	12 (6%)	1 (0%)	29	68
3	3	219/221 (99%)	204 (93%)	8 (4%)	7 (3%)	4	22
4	4	43/85 (51%)	37 (86%)	4 (9%)	2 (5%)	2	14
All	All	657/744 (88%)	606 (92%)	36 (6%)	15 (2%)	6	30

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	88	VAL
1	1	102	GLY
3	3	69	SER
3	3	131	HIS
3	3	197	ASP
1	1	210	LYS
2	2	171	GLY
3	3	219	SER
3	3	220	ARG
4	4	23	ASN
1	1	136	LYS
1	1	204	ASN
3	3	67	SER
3	3	194	HIS
4	4	22	ILE

### 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	1	162/182 (89%)	142 (88%)	20 (12%)	<b>4</b> <b>21</b>
2	2	180/192 (94%)	159 (88%)	21 (12%)	<b>5</b> <b>22</b>
3	3	184/184 (100%)	156 (85%)	28 (15%)	<b>3</b> <b>14</b>
4	4	37/67 (55%)	33 (89%)	4 (11%)	<b>6</b> <b>26</b>
All	All	563/625 (90%)	490 (87%)	73 (13%)	<b>4</b> <b>19</b>

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1	THR
1	1	12	THR
1	1	21	ASP
1	1	23	ARG
1	1	27	ARG
1	1	35	LEU
1	1	38	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	46	ASN
1	1	58	LYS
1	1	84	THR
1	1	85	ASN
1	1	101	VAL
1	1	113	THR
1	1	115	ARG
1	1	125	ARG
1	1	130	VAL
1	1	134	ASP
1	1	204	ASN
1	1	208	ARG
1	1	215	LYS
2	2	30	VAL
2	2	39	THR
2	2	48	THR
2	2	51	LEU
2	2	55	VAL
2	2	60	ARG
2	2	72	ASP
2	2	83	LEU
2	2	86	ASP
2	2	102	ARG
2	2	115	GLN
2	2	123	VAL
2	2	130	CYS
2	2	149	ASN
2	2	151	ARG
2	2	153	ASN
2	2	169	ASP
2	2	180	VAL
2	2	193	ILE
2	2	209	VAL
2	2	219	GLN
3	3	5	VAL
3	3	8	SER
3	3	25	VAL
3	3	29	VAL
3	3	40	ARG
3	3	42	THR
3	3	43	ASN
3	3	47	VAL

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Mol	Chain	Res	Type
3	3	63	VAL
3	3	68	ASN
3	3	76	CYS
3	3	79	LEU
3	3	104	THR
3	3	107	LEU
3	3	112	THR
3	3	115	THR
3	3	144	TYR
3	3	152	LEU
3	3	163	PHE
3	3	164	SER
3	3	185	VAL
3	3	193	THR
3	3	197	ASP
3	3	201	ILE
3	3	203	THR
3	3	213	ARG
3	3	219	SER
3	3	221	GLN
4	4	23	ASN
4	4	38	LEU
4	4	73	GLN
4	4	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	2	19	HIS
2	2	49	ASN
2	2	115	GLN
2	2	149	ASN
2	2	153	ASN
2	2	157	HIS
2	2	189	ASN
2	2	219	GLN
3	3	43	ASN
3	3	64	GLN
3	3	83	HIS
3	3	100	GLN
3	3	153	ASN
3	3	194	HIS

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Mol	Chain	Res	Type
4	4	23	ASN
4	4	32	ASN

### 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, 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	1	194/219 (88%)	-0.57	1 (0%) 91 75	4, 15, 71, 101	0
2	2	207/219 (94%)	-0.62	0 100 100	5, 14, 40, 93	0
3	3	221/221 (100%)	-0.54	0 100 100	5, 14, 76, 131	0
4	4	47/85 (55%)	-0.10	0 100 100	8, 39, 112, 119	0
All	All	669/744 (89%)	-0.54	1 (0%) 95 89	4, 15, 77, 131	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	134	ASP	2.6

### 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.