



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:23 PM GMT

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 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 <http://wwpdb.org/ValidationPDFNotes.html>

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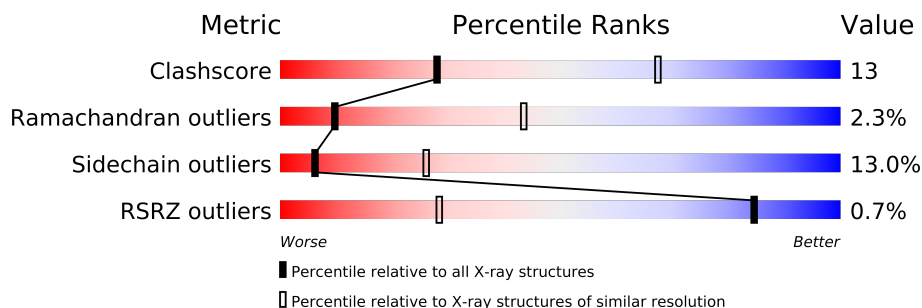
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	1	219	
2	2	219	
3	3	221	
4	4	85	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5210 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	1	194	Total	C	N	O	S	0	0	2
			1501	947	266	283	5			

- Molecule 2 is a protein called POLYPROTEIN.

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

- Molecule 3 is a protein called POLYPROTEIN.

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

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.

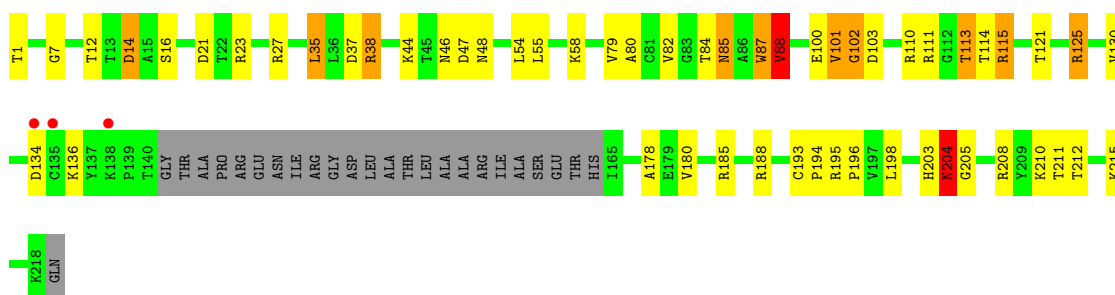
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	47	Total	C	N	O	S	0	0	1
			353	220	59	72	2			

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

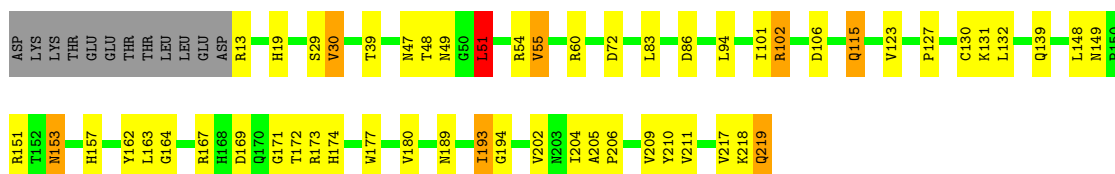
#### • Molecule 1: POLYPROTEIN

Chain 1: 



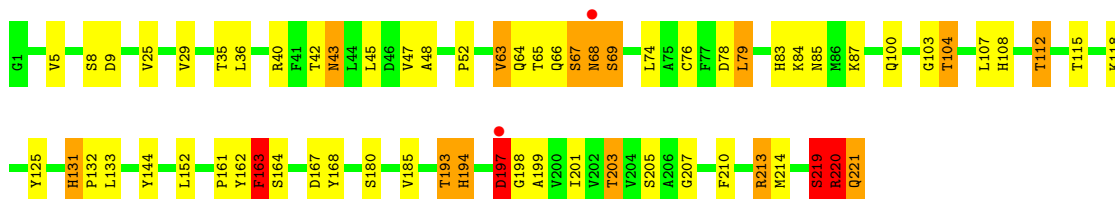
#### • Molecule 2: POLYPROTEIN

Chain 2: 



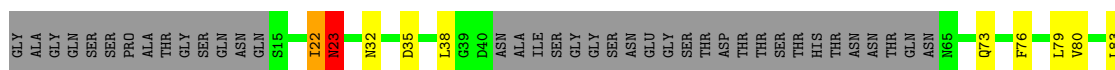
#### • Molecule 3: POLYPROTEIN

Chain 3: 



#### • Molecule 4: POLYPROTEIN

Chain 4: 





## 4 Data and refinement statistics

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) 54.9 (16.99-3.00)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.46 (at 3.02Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.230 , (Not available) 0.211 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 99.4	EDS
Estimated twinning fraction	0.248 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l 0.248 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.250 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 0.249 for 1/3*h+2/3*k-1/3*l,-k,-8/3*h-4/3*k-1/3*l 0.250 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 0.248 for -h,2/3*h+1/3*k+1/3*l,4/3*h+8/3*k-1/3*l 0.330 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.25$ , $\langle L^2 \rangle = 0.09$	Xtriage
Outliers	0 of 300765 reflections	Xtriage
$F_o, F_c$ correlation	0.54	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.

## 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	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:H	2:2:115:GLN:HE21	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:2:106:ASP:OD2	2:2:157:HIS:HE1	1.83	0.61
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:N	2:2:153:ASN:HD22	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
3:3:100:GLN:HE22	3:3:213:ARG:HH11	1.54	0.55
2:2:167:ARG:NH2	3:3:167:ASP:OD1	2.40	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
3:3:131:HIS:O	3:3:132:PRO:C	2.46	0.53
3:3:104:THR:HG23	3:3:207:GLY:HA3	1.90	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
3:3:64:GLN:CD	3:3:197:ASP:HB3	2.31	0.51
2:2:217:VAL:O	2:2:218:LYS:HB2	2.11	0.51
3:3:131:HIS:HB3	3:3:132:PRO:CD	2.40	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
3:3:163: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
3:3:65:THR:OG1	3:3:197:ASP:HA	2.11	0.49
1:1:211:THR:HG22	1:1:212:THR:N	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(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:HD1	3:3:163:PHE:N	2.12	0.47
3:3:104:THR:HG22	3:3:207:GLY:HA3	1.95	0.47
1:1:188:ARG:NH1	4:4:35:ASP:OD1	2.48	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:C	2:2:102:ARG:HD3	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
3:3:131:HIS:CB	3:3:132:PRO:CD	2.95	0.45
1:1:111:ARG:HD3	3:3:9:ASP:OD2	2.17	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:HD23	3:3:45:LEU:HA	1.78	0.43
3:3:52:PRO:HG3	3:3:205:SER:HB3	2.00	0.43
1:1:196:PRO:HB3	2:2:139:GLN:HB2	1.99	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:H	2:2:153:ASN:HD22	1.66	0.43
3:3:193:THR:O	3:3:194:HIS:HB2	2.19	0.43
1:1:14:ASP:HB2	1:1:16:SER:OG	2.19	0.43
3:3:131:HIS:O	3:3:133:LEU:N	2.52	0.43
3:3:78:ASP:OD1	3:3:180:SER:HB2	2.18	0.43
2:2:13:ARG:HD2	2:2:29:SER:O	2.19	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:HA	1:1:55:LEU:HD23	1.86	0.42
3:3:168:TYR:CD1	3:3:213:ARG:HD2	2.55	0.42
4:4:23:ASN:HD22	4:4:23:ASN:N	2.17	0.42
1:1:195:ARG:NH2	2:2:127:PRO:O	2.53	0.42
1:1:54:LEU:HD23	1:1:54:LEU:HA	1.72	0.41
1:1:35:LEU:O	1:1:38:ARG:CD	2.60	0.41
2:2:49:ASN:ND2	3:3:162:TYR:H	2.13	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:3:112:THR:O	3:3:112:THR:HG23	2.20	0.41
2:2:204:ILE:HG22	2:2:205:ALA:N	2.36	0.41
2:2:189:ASN:ND2	2:2:194:GLY:HA3	2.35	0.41
2:2:55:VAL:HG22	2:2:55:VAL:O	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
1:1:188:ARG:HD2	4:4:32:ASN:ND2	2.36	0.40
1:1:44:LYS:HA	1:1:180:VAL:O	2.21	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	1	190/219 (87%)	173 (91%)	12 (6%)	5 (3%)	8	39
2	2	205/219 (94%)	192 (94%)	12 (6%)	1 (0%)	38	84
3	3	219/221 (99%)	204 (93%)	8 (4%)	7 (3%)	6	33
4	4	43/85 (51%)	37 (86%)	4 (9%)	2 (5%)	4	21
All	All	657/744 (88%)	606 (92%)	36 (6%)	15 (2%)	10	43

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	88	VAL
1	1	102	GLY

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Mol	Chain	Res	Type
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 ⓘ

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%)	7	28
2	2	180/192 (94%)	159 (88%)	21 (12%)	8	31
3	3	184/184 (100%)	156 (85%)	28 (15%)	4	20
4	4	37/67 (55%)	33 (89%)	4 (11%)	9	35
All	All	563/625 (90%)	490 (87%)	73 (13%)	6	26

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
1	1	46	ASN
1	1	58	LYS

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Mol	Chain	Res	Type
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
3	3	63	VAL
3	3	68	ASN

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Mol	Chain	Res	Type
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

Some 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
4	4	23	ASN
4	4	32	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 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%)	0.22	3 (1%) 70 16	4, 15, 71, 101	0
2	2	207/219 (94%)	0.17	0 100 100	5, 14, 40, 93	0
3	3	221/221 (100%)	0.27	2 (0%) 81 24	5, 14, 76, 131	0
4	4	47/85 (55%)	0.53	0 100 100	8, 39, 112, 119	0
All	All	669/744 (89%)	0.24	5 (0%) 84 28	4, 15, 77, 131	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	138	LYS	3.1
1	1	134	ASP	2.5
3	3	68	ASN	2.3
1	1	135	CYS	2.3
3	3	197	ASP	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

There are no ligands in this entry.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.