



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:31 pm GMT

PDB ID : 1FMD  
Title : THE STRUCTURE AND ANTIGENICITY OF A TYPE C FOOT-AND-MOUTH DISEASE VIRUS  
Authors : Lea, S.; Fry, E.; Stuart, D.  
Deposited on : 1994-02-10  
Resolution : 3.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

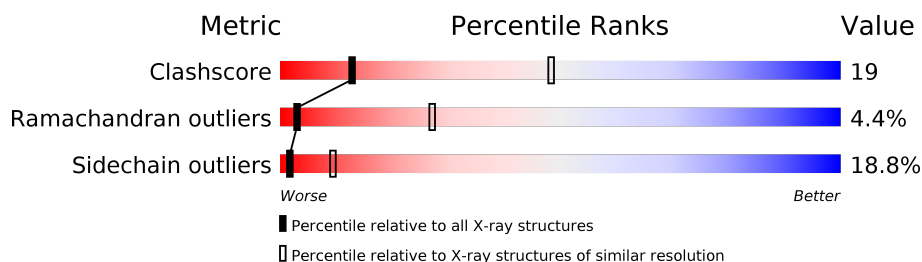
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	208	
2	2	218	
3	3	219	
4	4	85	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5168 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 FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	187	Total	C	N	O	S	0	0	0
			1445	913	259	270	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	46	ASP	GLY	CONFLICT	UNP Q65095
1	99	ASN	ASP	CONFLICT	UNP Q65095
1	112	VAL	LEU	CONFLICT	UNP Q65095
1	129	ALA	GLY	CONFLICT	UNP Q65095
1	144	ALA	THR	CONFLICT	UNP Q65095
1	153	THR	ALA	CONFLICT	UNP Q65095
1	155	HIS	ARG	CONFLICT	UNP Q65095
1	157	ALA	GLY	CONFLICT	UNP Q65095

- Molecule 2 is a protein called FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	218	Total	C	N	O	S	0	0	0
			1680	1061	296	316	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	21	HIS	GLN	CONFLICT	UNP Q9YQQ5
2	50	ALA	GLY	CONFLICT	UNP Q9YQQ5
2	122	LEU	GLN	CONFLICT	UNP Q9YQQ5
2	123	VAL	ALA	CONFLICT	UNP Q9YQQ5

- Molecule 3 is a protein called FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	219	Total	C	N	O	S	0	0	0
			1690	1075	277	327	11			

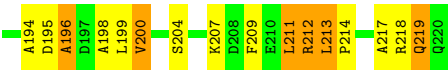
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	168	THR	ALA	CONFLICT	UNP Q9YQQ5

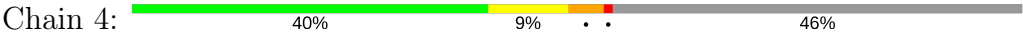
- Molecule 4 is a protein called FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP4).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	46	Total	C	N	O	S	0	0	0
			353	222	57	72	2			





● Molecule 4: FOOT-AND-MOUTH DISEASE VIRUS (SUBUNIT VP4)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	347.60 Å   347.60 Å   347.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	27.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (27.00-3.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.204 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

## 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	0.55	0/1480	0.86	4/2027 (0.2%)
2	2	0.54	0/1723	0.83	1/2352 (0.0%)
3	3	0.57	0/1739	0.88	1/2377 (0.0%)
4	4	0.70	0/359	1.00	2/481 (0.4%)
All	All	0.56	0/5301	0.87	8/7237 (0.1%)

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
3	3	0	1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	4	67	TRP	N-CA-C	7.23	130.53	111.00
4	4	66	ASP	C-N-CA	6.02	136.75	121.70
1	1	109	LYS	N-CA-C	-5.63	95.80	111.00
2	2	118	GLY	N-CA-C	-5.50	99.35	113.10
1	1	192	LEU	CA-CB-CG	5.38	127.69	115.30
3	3	188	GLN	N-CA-C	-5.36	96.52	111.00
1	1	81	THR	N-CA-C	-5.30	96.68	111.00
1	1	182	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	30	TYR	Sidechain



## 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	1	1445	0	1445	60	0
2	2	1680	0	1608	67	0
3	3	1690	0	1603	78	0
4	4	353	0	324	6	0
All	All	5168	0	4980	188	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 19.

All (188) 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)
2:2:48:THR:HG21	2:2:52:GLU:HB3	1.49	0.94
3:3:78:ASP:HB3	3:3:179:CYS:SG	2.13	0.87
1:1:70:THR:HG23	1:1:187:CYS:HB2	1.56	0.86
1:1:92:GLY:HA3	3:3:169:TYR:CE1	2.13	0.84
2:2:70:VAL:HG22	2:2:73:GLN:HE21	1.41	0.83
2:2:70:VAL:H	2:2:73:GLN:NE2	1.77	0.82
3:3:190:THR:HG22	3:3:191:HIS:H	1.45	0.80
2:2:58:ALA:HB3	2:2:208:VAL:HG21	1.63	0.80
1:1:203:GLN:HB2	1:1:204:PRO:HD2	1.69	0.75
3:3:103:GLY:HA3	3:3:209:PHE:HA	1.67	0.75
1:1:6:GLU:HG2	2:2:153:ASN:ND2	2.01	0.75
3:3:219:GLN:HA	3:3:219:GLN:NE2	2.00	0.74
3:3:52:PRO:HB3	3:3:204:SER:HB3	1.70	0.73
2:2:70:VAL:HG22	2:2:73:GLN:NE2	2.05	0.72
2:2:126:VAL:HG13	2:2:143:TYR:CE1	2.25	0.72
1:1:6:GLU:HB2	2:2:30:VAL:HG21	1.73	0.71
1:1:80:VAL:HG22	1:1:176:LEU:CD1	2.20	0.70
3:3:143:ILE:H	3:3:143:ILE:HD12	1.57	0.69
3:3:89:THR:HG23	3:3:92:ALA:H	1.58	0.67
3:3:190:THR:HG22	3:3:191:HIS:N	2.10	0.66
3:3:64:VAL:HG11	3:3:74:LEU:HB3	1.78	0.66
2:2:67:PHE:HB3	2:2:79:HIS:HD2	1.60	0.66
1:1:97:ALA:HB2	3:3:217:ALA:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:13:ASN:H	3:3:13:ASN:ND2	1.93	0.65
2:2:107:VAL:HG21	2:2:125:LEU:HD21	1.78	0.65
3:3:44:TYR:O	3:3:47:VAL:HG22	1.96	0.65
1:1:114:ARG:O	1:1:115:LEU:HD23	1.97	0.65
1:1:182:ARG:HH11	1:1:182:ARG:HG2	1.62	0.64
2:2:3:LYS:CB	2:2:12:ASP:HB2	2.28	0.64
2:2:70:VAL:O	2:2:73:GLN:HG2	1.98	0.64
1:1:122:PRO:HB3	3:3:100:GLN:HE21	1.63	0.63
3:3:78:ASP:CB	3:3:179:CYS:SG	2.84	0.63
1:1:107:TYR:HB2	3:3:14:MET:HB3	1.82	0.62
1:1:70:THR:HB	1:1:189:ARG:NH1	2.14	0.62
3:3:67:ARG:HE	3:3:72:ARG:NE	1.97	0.62
3:3:86:MET:O	3:3:88:ASN:N	2.32	0.62
1:1:89:VAL:HG13	1:1:93:ALA:HB3	1.81	0.62
1:1:182:ARG:HH11	1:1:182:ARG:CG	2.13	0.61
1:1:89:VAL:CG1	1:1:93:ALA:HB3	2.29	0.61
2:2:160:VAL:HG22	2:2:161:PRO:HD2	1.83	0.61
2:2:85:HIS:O	2:2:87:PRO:HD3	2.00	0.61
1:1:86:LEU:HD12	1:1:87:THR:N	2.15	0.61
1:1:86:LEU:HD11	1:1:168:VAL:HG13	1.82	0.61
1:1:196:PRO:HB3	1:1:201:HIS:HB2	1.84	0.60
3:3:191:HIS:CG	3:3:194:ALA:HB3	2.37	0.59
2:2:70:VAL:H	2:2:73:GLN:HE21	1.46	0.59
1:1:122:PRO:HB3	3:3:100:GLN:NE2	2.17	0.59
3:3:185:CYS:HB2	3:3:187:TYR:CE1	2.38	0.59
3:3:195:ASP:O	3:3:196:ALA:HB3	2.02	0.59
1:1:70:THR:HG22	1:1:189:ARG:HG2	1.84	0.59
3:3:187:TYR:CD1	3:3:187:TYR:N	2.70	0.59
3:3:78:ASP:OD2	3:3:179:CYS:SG	2.62	0.58
3:3:63:TYR:HA	3:3:200:VAL:HA	1.84	0.58
3:3:212:ARG:HD3	3:3:213:LEU:HD22	1.86	0.57
1:1:92:GLY:HA3	3:3:169:TYR:HE1	1.66	0.57
3:3:14:MET:HG3	3:3:15:VAL:N	2.18	0.57
3:3:135:ASN:N	3:3:135:ASN:HD22	2.04	0.56
3:3:94:LEU:HD12	3:3:211:LEU:HD23	1.88	0.56
3:3:102:THR:HA	3:3:161:TYR:CE2	2.40	0.56
1:1:78:ILE:HG22	1:1:178:VAL:HG12	1.88	0.56
2:2:126:VAL:HG13	2:2:143:TYR:CD1	2.41	0.55
1:1:61:ILE:HG23	1:1:62:VAL:N	2.21	0.55
2:2:114:ASN:ND2	2:2:116:PHE:H	2.04	0.55
3:3:120:ARG:HH11	3:3:146:GLU:HG2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:102:THR:HA	3:3:161:TYR:CD2	2.41	0.55
1:1:129:ALA:O	1:1:130:TYR:HB2	2.07	0.54
2:2:70:VAL:N	2:2:73:GLN:NE2	2.53	0.54
3:3:121:TYR:CE2	3:3:199:LEU:HD22	2.43	0.54
3:3:93:GLY:O	3:3:96:GLN:HG2	2.08	0.54
1:1:89:VAL:HG13	1:1:93:ALA:CB	2.38	0.53
3:3:161:TYR:CE1	3:3:163:SER:HB3	2.42	0.53
1:1:105:THR:O	3:3:15:VAL:HA	2.09	0.53
2:2:115:GLN:HE21	2:2:115:GLN:N	2.07	0.53
3:3:135:ASN:H	3:3:135:ASN:HD22	1.54	0.53
1:1:92:GLY:CA	3:3:169:TYR:CE1	2.89	0.53
3:3:167:TYR:CE2	3:3:212:ARG:HG2	2.43	0.53
2:2:54:ARG:HE	2:2:56:HIS:CD2	2.27	0.52
2:2:58:ALA:CB	2:2:208:VAL:HG21	2.37	0.52
1:1:86:LEU:CD1	1:1:168:VAL:HG13	2.39	0.52
3:3:191:HIS:HB2	3:3:194:ALA:HB3	1.91	0.52
3:3:97:TYR:O	3:3:214:PRO:HA	2.10	0.52
3:3:107:LEU:HD23	3:3:159:ILE:HD11	1.91	0.51
2:2:26:THR:HG22	2:2:28:SER:H	1.76	0.51
1:1:6:GLU:HG2	2:2:153:ASN:HD21	1.75	0.51
3:3:79:VAL:HG23	3:3:183:TRP:HA	1.91	0.51
1:1:73:PHE:CD1	1:1:74:SER:N	2.79	0.51
2:2:118:GLY:H	2:2:188:THR:HB	1.76	0.51
2:2:64:MET:O	2:2:64:MET:HG3	2.10	0.51
3:3:73:LEU:HD21	3:3:76:LYS:HB3	1.92	0.51
3:3:89:THR:CG2	3:3:92:ALA:H	2.24	0.50
3:3:89:THR:HG22	3:3:92:ALA:CB	2.41	0.50
1:1:73:PHE:C	1:1:73:PHE:CD1	2.85	0.50
3:3:212:ARG:O	3:3:213:LEU:HB2	2.11	0.50
3:3:89:THR:HG22	3:3:92:ALA:HB3	1.92	0.50
1:1:82:HIS:CE1	1:1:86:LEU:HB2	2.46	0.50
2:2:115:GLN:NE2	2:2:115:GLN:H	2.08	0.50
3:3:168:THR:HG22	3:3:169:TYR:N	2.27	0.50
2:2:166:ASN:HD22	3:3:165:ALA:HA	1.77	0.50
2:2:114:ASN:HD21	2:2:116:PHE:HB2	1.77	0.49
2:2:12:ASP:O	2:2:13:ARG:HB2	2.12	0.49
2:2:48:THR:HG22	2:2:48:THR:O	2.13	0.49
2:2:214:LEU:HB3	2:2:215:PRO:HD2	1.94	0.49
1:1:7:SER:O	1:1:8:ALA:HB3	2.13	0.49
3:3:102:THR:HG22	3:3:103:GLY:N	2.28	0.49
3:3:43:ASN:HD21	3:3:45:LEU:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:161:TYR:C	3:3:161:TYR:CD1	2.86	0.48
1:1:80:VAL:HG21	1:1:86:LEU:HD21	1.96	0.48
3:3:219:GLN:HA	3:3:219:GLN:HE21	1.76	0.48
3:3:78:ASP:HB3	3:3:179:CYS:HG	1.78	0.48
3:3:67:ARG:HH21	3:3:72:ARG:HD3	1.78	0.48
2:2:126:VAL:HG13	2:2:127:PRO:HD2	1.95	0.47
1:1:130:TYR:CE2	2:2:174:HIS:HD2	2.32	0.47
2:2:70:VAL:HG23	2:2:72:SER:H	1.78	0.47
1:1:127:ALA:HB3	1:1:163:PHE:HE2	1.79	0.47
2:2:42:SER:HB3	4:4:38:LEU:HD21	1.96	0.47
1:1:130:TYR:CZ	2:2:174:HIS:CD2	3.03	0.47
3:3:190:THR:CG2	3:3:191:HIS:H	2.22	0.47
3:3:195:ASP:O	3:3:196:ALA:CB	2.62	0.47
1:1:182:ARG:HH11	1:1:182:ARG:HB3	1.80	0.47
3:3:104:THR:CG2	3:3:158:SER:HB3	2.45	0.46
3:3:104:THR:HG23	3:3:158:SER:HB3	1.97	0.46
2:2:120:CYS:O	2:2:184:VAL:HG22	2.16	0.46
2:2:162:TYR:C	2:2:162:TYR:CD1	2.89	0.46
2:2:166:ASN:ND2	3:3:165:ALA:HA	2.30	0.46
3:3:190:THR:CG2	3:3:191:HIS:N	2.79	0.46
1:1:90:PRO:HG2	3:3:99:THR:HG21	1.98	0.46
1:1:36:LEU:HD11	1:1:185:LEU:HD11	1.97	0.46
1:1:49:HIS:CE1	1:1:55:GLN:HE22	2.34	0.46
2:2:115:GLN:NE2	2:2:115:GLN:N	2.64	0.46
2:2:118:GLY:N	2:2:188:THR:HB	2.31	0.46
3:3:123:VAL:HG12	3:3:147:TRP:HZ3	1.81	0.46
3:3:168:THR:HG22	3:3:169:TYR:H	1.81	0.46
2:2:33:THR:HB	2:2:158:ILE:HG12	1.96	0.46
3:3:211:LEU:HD12	3:3:211:LEU:HA	1.81	0.46
2:2:48:THR:C	2:2:50:ALA:N	2.69	0.45
2:2:132:ILE:HD13	2:2:137:LYS:HG2	1.98	0.45
2:2:61:PHE:HA	2:2:203:ILE:O	2.16	0.45
4:4:34:MET:HA	4:4:34:MET:HE3	1.98	0.45
1:1:130:TYR:CE2	2:2:174:HIS:CD2	3.05	0.44
1:1:86:LEU:HD12	1:1:86:LEU:C	2.37	0.44
2:2:54:ARG:NH1	2:2:207:ASN:HA	2.32	0.44
3:3:77:PHE:O	3:3:183:TRP:HB3	2.17	0.44
4:4:66:ASP:HA	4:4:70:LYS:HE3	2.00	0.44
1:1:77:GLU:HB3	1:1:179:ARG:HB3	1.99	0.44
1:1:25:GLN:NE2	1:1:25:GLN:H	2.16	0.44
2:2:70:VAL:N	2:2:73:GLN:HE21	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:73:GLN:OE1	2:2:77:HIS:CE1	2.71	0.44
1:1:61:ILE:CG2	1:1:62:VAL:N	2.81	0.43
3:3:15:VAL:HG12	3:3:17:THR:H	1.82	0.43
1:1:98:LEU:HG	1:1:169:LYS:HB2	1.99	0.43
1:1:197:THR:HG23	1:1:198:GLY:H	1.83	0.43
2:2:188:THR:HG22	2:2:190:ASN:ND2	2.33	0.43
3:3:100:GLN:HA	3:3:168:THR:O	2.19	0.43
3:3:74:LEU:HD11	3:3:188:GLN:HB2	2.00	0.43
1:1:80:VAL:HG22	1:1:176:LEU:HD11	1.98	0.43
1:1:129:ALA:HB3	1:1:189:ARG:NH1	2.34	0.43
2:2:214:LEU:HD23	3:3:127:PRO:HG2	1.99	0.43
4:4:76:PHE:HE2	4:4:80:PHE:HD2	1.67	0.43
1:1:61:ILE:HG23	1:1:62:VAL:HG23	2.01	0.43
1:1:103:ASN:O	1:1:105:THR:N	2.52	0.42
1:1:69:ALA:C	1:1:189:ARG:HG3	2.40	0.42
2:2:118:GLY:CA	2:2:188:THR:HB	2.49	0.42
4:4:66:ASP:O	4:4:69:SER:HB3	2.20	0.42
2:2:69:TRP:CE2	2:2:187:LEU:HB2	2.54	0.42
2:2:217:LYS:HB3	2:2:217:LYS:HE2	1.81	0.42
1:1:104:PRO:HG3	3:3:17:THR:HG21	2.02	0.42
1:1:14:THR:HB	1:1:16:GLU:OE1	2.19	0.42
2:2:173:GLN:O	2:2:174:HIS:HB2	2.20	0.42
2:2:137:LYS:O	2:2:140:LEU:HB2	2.20	0.41
2:2:48:THR:O	2:2:50:ALA:N	2.52	0.41
1:1:131:THR:OG1	2:2:128:GLU:HA	2.21	0.41
1:1:192:LEU:HD21	2:2:136:GLU:HB3	2.03	0.41
2:2:62:PHE:CD1	2:2:62:PHE:C	2.94	0.41
3:3:111:PHE:CZ	3:3:113:GLY:HA3	2.55	0.41
3:3:112:THR:HB	3:3:198:ALA:O	2.20	0.41
1:1:186:TYR:N	1:1:186:TYR:CD1	2.88	0.41
2:2:67:PHE:HB3	2:2:79:HIS:CD2	2.49	0.41
1:1:182:ARG:CB	1:1:182:ARG:HH11	2.34	0.41
2:2:54:ARG:HB2	2:2:209:HIS:NE2	2.36	0.41
2:2:82:VAL:HB	2:2:175:ARG:NH1	2.36	0.41
3:3:17:THR:HG23	3:3:17:THR:O	2.21	0.41
4:4:25:TYR:C	4:4:25:TYR:CD1	2.94	0.41
2:2:45:GLY:HA3	2:2:167:ARG:HE	1.85	0.40
2:2:48:THR:HB	2:2:52:GLU:OE1	2.21	0.40
3:3:143:ILE:HD12	3:3:143:ILE:N	2.31	0.40
1:1:131:THR:HG21	2:2:129:MET:O	2.20	0.40
2:2:54:ARG:HB2	2:2:209:HIS:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:190:THR:O	3:3:191:HIS:HB3	2.22	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	183/208 (88%)	158 (86%)	17 (9%)	8 (4%)	3	27
2	2	216/218 (99%)	177 (82%)	29 (13%)	10 (5%)	3	26
3	3	217/219 (99%)	182 (84%)	25 (12%)	10 (5%)	3	26
4	4	42/85 (49%)	36 (86%)	5 (12%)	1 (2%)	7	42
All	All	658/730 (90%)	553 (84%)	76 (12%)	29 (4%)	3	27

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	6	GLU
2	2	35	GLY
2	2	174	HIS
3	3	87	SER
3	3	219	GLN
4	4	67	TRP
2	2	49	SER
2	2	173	GLN
3	3	14	MET
3	3	59	ASN
3	3	71	GLN
1	1	193	PRO
1	1	104	PRO
1	1	130	TYR

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Mol	Chain	Res	Type
1	1	187	CYS
2	2	85	HIS
2	2	190	ASN
3	3	196	ALA
1	1	111	PRO
2	2	131	ASP
2	2	176	PRO
3	3	15	VAL
3	3	83	ALA
1	1	61	ILE
3	3	24	PRO
3	3	180	VAL
1	1	32	VAL
1	1	122	PRO
2	2	87	PRO

### 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	157/173 (91%)	130 (83%)	27 (17%)	2	13
2	2	177/187 (95%)	143 (81%)	34 (19%)	1	9
3	3	177/177 (100%)	141 (80%)	36 (20%)	1	7
4	4	37/67 (55%)	31 (84%)	6 (16%)	3	16
All	All	548/604 (91%)	445 (81%)	103 (19%)	2	9

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	THR
1	1	3	THR
1	1	4	THR
1	1	24	VAL
1	1	25	GLN
1	1	27	ARG

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Mol	Chain	Res	Type
1	1	30	THR
1	1	42	VAL
1	1	70	THR
1	1	81	THR
1	1	86	LEU
1	1	89	VAL
1	1	98	LEU
1	1	101	THR
1	1	122	PRO
1	1	128	THR
1	1	131	THR
1	1	158	HIS
1	1	172	THR
1	1	179	ARG
1	1	182	ARG
1	1	189	ARG
1	1	191	ILE
1	1	197	THR
1	1	200	ARG
1	1	205	LEU
1	1	210	LYS
2	2	12	ASP
2	2	23	THR
2	2	32	VAL
2	2	43	THR
2	2	49	SER
2	2	52	GLU
2	2	53	THR
2	2	55	VAL
2	2	63	LYS
2	2	66	LEU
2	2	90	VAL
2	2	94	LEU
2	2	97	SER
2	2	102	ARG
2	2	114	ASN
2	2	115	GLN
2	2	120	CYS
2	2	123	VAL
2	2	131	ASP
2	2	133	SER
2	2	134	ASP

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Mol	Chain	Res	Type
2	2	149	ASN
2	2	151	ARG
2	2	153	ASN
2	2	154	MET
2	2	160	VAL
2	2	162	TYR
2	2	169	ASP
2	2	170	GLN
2	2	172	LYS
2	2	175	ARG
2	2	180	VAL
2	2	191	THR
2	2	196	GLN
3	3	13	ASN
3	3	17	THR
3	3	35	THR
3	3	40	ARG
3	3	42	THR
3	3	45	LEU
3	3	53	THR
3	3	56	MET
3	3	58	GLU
3	3	59	ASN
3	3	69	ASP
3	3	76	LYS
3	3	78	ASP
3	3	89	THR
3	3	100	GLN
3	3	101	TYR
3	3	107	LEU
3	3	112	THR
3	3	130	MET
3	3	135	ASN
3	3	153	SER
3	3	161	TYR
3	3	177	THR
3	3	179	CYS
3	3	180	VAL
3	3	183	TRP
3	3	185	CYS
3	3	186	VAL
3	3	187	TYR

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Mol	Chain	Res	Type
3	3	191	HIS
3	3	200	VAL
3	3	207	LYS
3	3	211	LEU
3	3	212	ARG
3	3	213	LEU
3	3	218	ARG
4	4	35	ASP
4	4	37	GLN
4	4	38	LEU
4	4	66	ASP
4	4	73	SER
4	4	76	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	25	GLN
1	1	55	GLN
2	2	56	HIS
2	2	73	GLN
2	2	114	ASN
2	2	115	GLN
2	2	149	ASN
2	2	153	ASN
2	2	166	ASN
3	3	13	ASN
3	3	43	ASN
3	3	100	GLN
3	3	135	ASN
3	3	152	ASN
3	3	191	HIS
3	3	219	GLN
4	4	31	GLN
4	4	32	ASN

### 5.3.3 RNA ⓘ

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 carbohydrates 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.