



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 10:33 am GMT

PDB ID : 2D7S  
Title : Foot and Mouth Disease Virus RNA-dependent RNA polymerase in complex with VPg protein  
Authors : Ferrer-Orta, C.; Arias, A.; Perez-Luque, R.; Escarmis, C.; Domingo, E.; Verdaguier, N.  
Deposited on : 2005-11-29  
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

<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

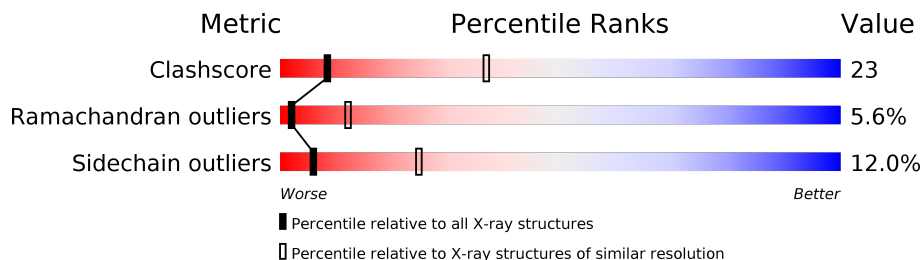
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (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. 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	A	474	
2	B	23	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3855 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 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3737	2375	646	695	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	ALA	-	CLONING ARTIFACT	GB 6318192
A	472	ALA	-	CLONING ARTIFACT	GB 6318192
A	473	LEU	-	CLONING ARTIFACT	GB 6318192
A	474	GLU	-	CLONING ARTIFACT	GB 6318192

- Molecule 2 is a protein called VPg1 protein.

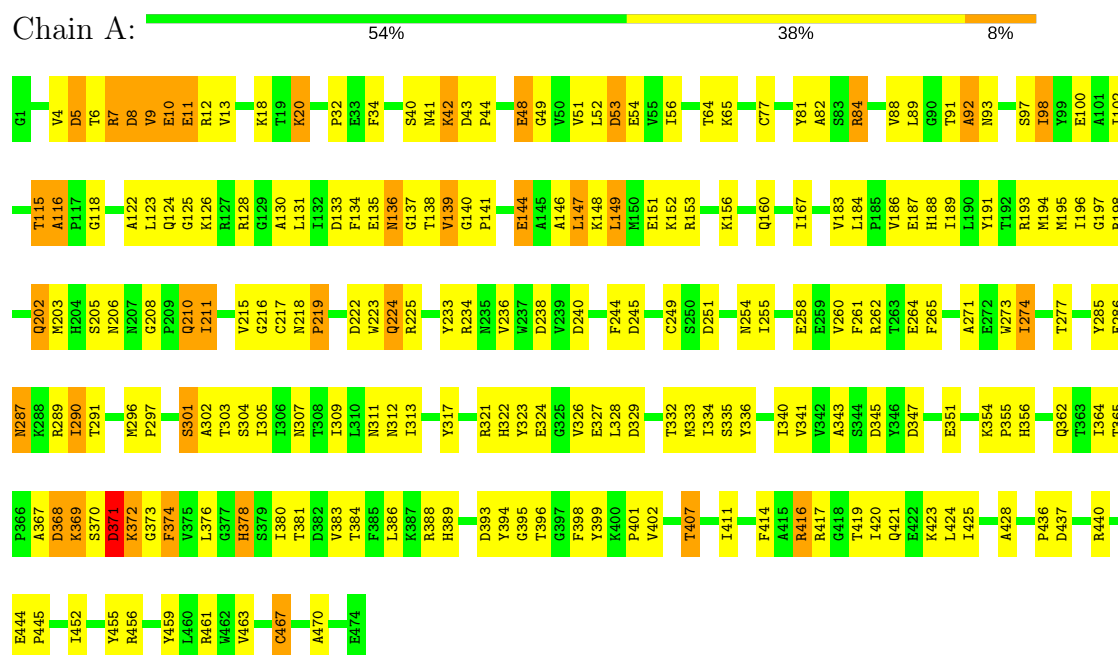
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	0	0	0
			118	76	23	19			

### 3 Residue-property plots [i](#)

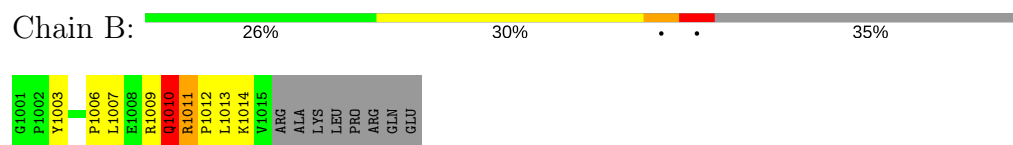
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

#### • Molecule 1: RNA-dependent RNA polymerase



#### • Molecule 2: VPg1 protein



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.09 Å 95.09 Å 100.63 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.74 – 3.00	Depositor
% Data completeness (in resolution range)	99.9 (29.74-3.00)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.277 , 0.294	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3855	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

## 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	0.30	0/3826	0.61	1/5182 (0.0%)
2	B	0.33	0/121	0.91	0/163
All	All	0.30	0/3947	0.63	1/5345 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	GLY	N-CA-C	5.04	125.69	113.10

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	3737	0	3658	173	0
2	B	118	0	124	10	0
All	All	3855	0	3782	176	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 23.

All (176) 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:416:ARG:HB2	1:A:416:ARG:HH11	1.17	1.03
1:A:351:GLU:HG2	1:A:374:PHE:HB2	1.44	0.97
1:A:416:ARG:HB2	1:A:416:ARG:NH1	1.91	0.85
1:A:211:ILE:H	1:A:211:ILE:HD13	1.42	0.83
1:A:211:ILE:N	1:A:211:ILE:HD13	1.97	0.79
1:A:407:THR:HG23	2:B:1007:LEU:HD23	1.64	0.79
1:A:147:LEU:O	1:A:151:GLU:HG3	1.82	0.78
1:A:274:ILE:HD13	1:A:274:ILE:O	1.87	0.75
1:A:211:ILE:H	1:A:211:ILE:CD1	1.99	0.75
1:A:251:ASP:O	1:A:255:ILE:HD13	1.87	0.74
1:A:216:GLY:H	2:B:1011:ARG:NH2	1.85	0.73
1:A:322:HIS:HB2	1:A:356:HIS:CE1	2.24	0.73
1:A:388:ARG:HD3	1:A:401:PRO:HB2	1.69	0.73
1:A:340:ILE:HD12	1:A:341:VAL:H	1.53	0.72
1:A:333:MET:HE3	1:A:340:ILE:HD13	1.72	0.72
1:A:354:LYS:HG2	1:A:364:ILE:HD11	1.70	0.72
1:A:273:TRP:O	1:A:277:THR:HG23	1.90	0.71
1:A:122:ALA:C	1:A:124:GLN:H	1.94	0.71
1:A:152:LYS:O	1:A:153:ARG:HB2	1.92	0.69
1:A:92:ALA:O	1:A:198:ARG:HG2	1.92	0.69
1:A:148:LYS:HG3	1:A:151:GLU:OE1	1.92	0.69
1:A:238:ASP:HB2	1:A:383:VAL:HG12	1.75	0.68
1:A:52:LEU:O	1:A:56:ILE:HD13	1.94	0.67
1:A:296:MET:HG2	1:A:297:PRO:HD2	1.78	0.66
1:A:84:ARG:HG2	1:A:328:LEU:HD13	1.78	0.65
1:A:254:ASN:O	1:A:258:GLU:HG3	1.97	0.64
1:A:146:ALA:HA	1:A:149:LEU:HG	1.78	0.64
1:A:167:ILE:HD11	1:A:414:PHE:HB2	1.79	0.63
1:A:102:ILE:HD12	1:A:137:GLY:O	2.00	0.62
1:A:98:ILE:O	1:A:102:ILE:HG13	1.99	0.62
1:A:303:THR:HG23	1:A:304:SER:N	2.14	0.62
1:A:305:ILE:O	1:A:309:ILE:HD13	2.00	0.62
1:A:335:SER:HB3	1:A:340:ILE:HD13	1.82	0.62
1:A:130:ALA:O	1:A:131:LEU:HD12	2.00	0.61
1:A:411:ILE:CG1	2:B:1007:LEU:HD21	2.29	0.61
1:A:13:VAL:O	1:A:286:GLU:HA	2.01	0.61
1:A:354:LYS:HB2	1:A:355:PRO:HD3	1.83	0.60
2:B:1010:GLN:O	2:B:1011:ARG:HB2	2.02	0.59
1:A:303:THR:HG23	1:A:304:SER:H	1.66	0.59
1:A:262:ARG:HH11	1:A:262:ARG:HG2	1.68	0.59
1:A:452:ILE:N	1:A:452:ILE:HD12	2.18	0.58
1:A:234:ARG:HG2	1:A:345:ASP:OD1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:O	1:A:249:CYS:HB2	2.04	0.58
1:A:351:GLU:OE1	1:A:373:GLY:HA2	2.02	0.58
1:A:77:CYS:SG	1:A:317:TYR:HA	2.43	0.58
1:A:234:ARG:HH11	1:A:234:ARG:HG3	1.69	0.57
1:A:9:VAL:HG12	1:A:289:ARG:HD2	1.86	0.57
1:A:102:ILE:HD12	1:A:137:GLY:C	2.24	0.57
1:A:333:MET:HE3	1:A:340:ILE:CD1	2.34	0.57
1:A:147:LEU:HD22	1:A:147:LEU:O	2.05	0.56
1:A:196:ILE:HG21	1:A:261:PHE:CE2	2.40	0.56
1:A:424:LEU:O	1:A:428:ALA:HB2	2.05	0.56
1:A:82:ALA:HB2	1:A:260:VAL:HG22	1.87	0.55
1:A:140:GLY:O	1:A:144:GLU:HG3	2.06	0.55
1:A:301:SER:O	1:A:302:ALA:HB3	2.07	0.55
1:A:133:ASP:HB3	1:A:136:ASN:HB2	1.88	0.54
1:A:233:TYR:CD1	1:A:233:TYR:N	2.74	0.54
1:A:215:VAL:HA	1:A:336:TYR:CE1	2.43	0.54
1:A:4:VAL:HG22	1:A:291:THR:HB	1.89	0.54
1:A:167:ILE:HB	2:B:1007:LEU:HD12	1.89	0.54
1:A:389:HIS:HB3	1:A:402:VAL:HG23	1.90	0.54
1:A:81:TYR:CD2	1:A:313:ILE:HD11	2.43	0.53
1:A:389:HIS:HB3	1:A:402:VAL:CG2	2.39	0.53
1:A:91:THR:C	1:A:93:ASN:H	2.11	0.53
1:A:4:VAL:CG2	1:A:291:THR:HB	2.38	0.53
2:B:1010:GLN:HG2	2:B:1010:GLN:O	2.09	0.53
1:A:388:ARG:HD3	1:A:401:PRO:CB	2.39	0.53
2:B:1010:GLN:O	2:B:1010:GLN:CG	2.56	0.53
1:A:122:ALA:C	1:A:124:GLN:N	2.63	0.52
1:A:84:ARG:HD3	1:A:84:ARG:O	2.09	0.52
1:A:217:CYS:HB2	1:A:222:ASP:OD2	2.10	0.52
1:A:419:THR:HG22	1:A:423:LYS:HD3	1.91	0.52
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.09	0.51
1:A:4:VAL:O	1:A:5:ASP:HB2	2.09	0.51
1:A:262:ARG:NH1	1:A:262:ARG:HG2	2.25	0.51
1:A:376:LEU:HD12	1:A:376:LEU:N	2.26	0.51
1:A:411:ILE:HG12	2:B:1007:LEU:HD21	1.91	0.51
1:A:322:HIS:ND1	1:A:356:HIS:HE1	2.09	0.51
1:A:364:ILE:O	1:A:364:ILE:HD12	2.11	0.50
1:A:184:LEU:HD23	1:A:188:HIS:CD2	2.46	0.50
1:A:381:THR:C	1:A:389:HIS:HE1	2.15	0.50
1:A:368:ASP:O	1:A:370:SER:N	2.45	0.50
1:A:416:ARG:NH2	1:A:417:ARG:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:O	1:A:260:VAL:HG12	2.12	0.49
1:A:196:ILE:HG21	1:A:261:PHE:CD2	2.49	0.48
1:A:128:ARG:HB3	1:A:134:PHE:HE2	1.78	0.48
1:A:321:ARG:HH11	1:A:356:HIS:HD2	1.60	0.48
1:A:354:LYS:N	1:A:355:PRO:CD	2.76	0.48
1:A:371:ASP:O	1:A:373:GLY:N	2.46	0.48
1:A:332:THR:HG22	1:A:343:ALA:HB3	1.96	0.48
1:A:340:ILE:HD12	1:A:341:VAL:N	2.27	0.48
1:A:65:LYS:HE3	1:A:65:LYS:HA	1.96	0.48
1:A:184:LEU:HD12	1:A:184:LEU:N	2.30	0.47
1:A:312:ASN:HA	1:A:333:MET:HE1	1.97	0.47
1:A:32:PRO:C	1:A:34:PHE:H	2.18	0.47
1:A:208:GLY:N	1:A:211:ILE:HD11	2.30	0.47
1:A:334:ILE:O	1:A:334:ILE:HG23	2.14	0.47
1:A:203:MET:HA	1:A:203:MET:HE2	1.97	0.47
1:A:216:GLY:N	2:B:1011:ARG:NH2	2.59	0.47
1:A:191:TYR:O	1:A:195:MET:HG2	2.15	0.46
1:A:402:VAL:HG23	1:A:402:VAL:O	2.15	0.46
1:A:91:THR:HB	1:A:265:PHE:O	2.16	0.46
1:A:322:HIS:HD2	1:A:323:TYR:CE1	2.34	0.46
1:A:381:THR:C	1:A:389:HIS:CE1	2.89	0.46
1:A:41:ASN:N	1:A:41:ASN:OD1	2.48	0.46
1:A:440:ARG:O	1:A:444:GLU:N	2.47	0.46
1:A:100:GLU:C	1:A:102:ILE:H	2.18	0.46
1:A:321:ARG:HG2	1:A:356:HIS:CD2	2.51	0.46
1:A:186:VAL:O	1:A:186:VAL:HG22	2.16	0.46
1:A:271:ALA:O	1:A:274:ILE:HG22	2.16	0.46
1:A:89:LEU:HD11	1:A:203:MET:CE	2.47	0.45
1:A:206:ASN:O	1:A:211:ILE:CD1	2.65	0.45
1:A:262:ARG:HB3	1:A:264:GLU:OE2	2.17	0.45
1:A:89:LEU:HD11	1:A:203:MET:HE3	1.97	0.45
1:A:436:PRO:HG3	1:A:455:TYR:CE2	2.52	0.45
1:A:51:VAL:HB	1:A:54:GLU:HB2	1.98	0.45
1:A:332:THR:CG2	1:A:343:ALA:HB3	2.47	0.45
1:A:233:TYR:H	1:A:233:TYR:HD1	1.65	0.45
1:A:236:VAL:HG12	1:A:383:VAL:HG11	1.99	0.45
1:A:421:GLN:O	1:A:425:ILE:HG13	2.17	0.45
1:A:13:VAL:O	1:A:286:GLU:HG2	2.17	0.45
1:A:40:SER:OG	1:A:42:LYS:HG3	2.17	0.45
1:A:371:ASP:C	1:A:371:ASP:OD1	2.54	0.45
1:A:10:GLU:HG3	1:A:11:GLU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ASP:C	1:A:370:SER:H	2.20	0.44
1:A:6:THR:HA	1:A:290:ILE:HG23	1.99	0.44
1:A:40:SER:C	1:A:42:LYS:H	2.21	0.44
1:A:98:ILE:HD13	1:A:194:MET:SD	2.58	0.44
1:A:393:ASP:C	1:A:395:GLY:H	2.22	0.44
1:A:354:LYS:HG2	1:A:364:ILE:CD1	2.42	0.44
1:A:364:ILE:HD13	1:A:374:PHE:CE1	2.53	0.44
1:A:467:CYS:HB3	1:A:470:ALA:HB3	1.99	0.44
1:A:97:SER:O	1:A:98:ILE:C	2.56	0.44
1:A:370:SER:O	1:A:372:LYS:N	2.51	0.43
1:A:444:GLU:HB3	1:A:445:PRO:HD3	2.00	0.43
1:A:156:LYS:HD3	1:A:156:LYS:HA	1.76	0.43
1:A:53:ASP:OD2	1:A:285:TYR:HE2	2.00	0.43
1:A:354:LYS:HA	1:A:364:ILE:HD11	2.00	0.43
1:A:12:ARG:HA	1:A:287:ASN:HA	2.01	0.43
1:A:144:GLU:HA	1:A:147:LEU:HB3	2.00	0.43
1:A:217:CYS:O	2:B:1011:ARG:HD2	2.19	0.43
1:A:224:GLN:OE1	1:A:399:TYR:HD2	2.02	0.43
1:A:144:GLU:HG3	1:A:144:GLU:H	1.54	0.42
1:A:139:VAL:HB	1:A:140:GLY:H	1.45	0.42
1:A:340:ILE:CG1	1:A:341:VAL:N	2.82	0.42
1:A:89:LEU:HD22	1:A:202:GLN:HB3	2.02	0.42
1:A:210:GLN:HA	1:A:210:GLN:OE1	2.20	0.42
1:A:459:TYR:O	1:A:463:VAL:HG23	2.19	0.42
1:A:92:ALA:O	1:A:198:ARG:CG	2.65	0.42
1:A:396:THR:HB	1:A:398:PHE:CD2	2.55	0.42
1:A:146:ALA:CA	1:A:149:LEU:HG	2.47	0.42
1:A:340:ILE:HG13	1:A:341:VAL:N	2.34	0.42
1:A:43:ASP:HA	1:A:44:PRO:HD3	1.93	0.42
1:A:245:ASP:OD1	1:A:307:ASN:ND2	2.54	0.41
1:A:13:VAL:H	1:A:286:GLU:C	2.23	0.41
1:A:187:GLU:HG2	1:A:188:HIS:N	2.35	0.41
1:A:467:CYS:HB3	1:A:470:ALA:CB	2.50	0.41
1:A:7:ARG:HG3	1:A:8:ASP:N	2.34	0.41
1:A:160:GLN:HB3	1:A:183:VAL:O	2.21	0.41
1:A:193:ARG:O	1:A:197:GLY:HA3	2.20	0.41
1:A:364:ILE:HG13	1:A:364:ILE:H	1.72	0.41
1:A:218:ASN:HA	1:A:219:PRO:HD2	1.87	0.41
1:A:115:THR:O	1:A:116:ALA:C	2.58	0.41
1:A:189:ILE:O	1:A:193:ARG:HG2	2.20	0.41
1:A:371:ASP:O	1:A:372:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HE2	1:A:20:LYS:HB3	1.94	0.41
1:A:234:ARG:HH11	1:A:234:ARG:CG	2.34	0.41
1:A:416:ARG:HG3	1:A:419:THR:OG1	2.21	0.41
1:A:118:GLY:HA2	1:A:160:GLN:HE21	1.86	0.40
1:A:347:ASP:HB3	1:A:376:LEU:CD2	2.51	0.40
1:A:386:LEU:O	1:A:388:ARG:HG3	2.21	0.40
1:A:364:ILE:HD13	1:A:374:PHE:HE1	1.86	0.40
1:A:186:VAL:O	1:A:186:VAL:CG2	2.69	0.40
1:A:20:LYS:O	1:A:416:ARG:HA	2.21	0.40
1:A:393:ASP:HB3	1:A:398:PHE:O	2.21	0.40
1:A:244:PHE:HA	1:A:362:GLN:HE22	1.85	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	A	472/474 (100%)	393 (83%)	56 (12%)	23 (5%)	2	15
2	B	13/23 (56%)	5 (38%)	4 (31%)	4 (31%)	0	0
All	All	485/497 (98%)	398 (82%)	60 (12%)	27 (6%)	2	12

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	VAL
1	A	369	LYS
1	A	371	ASP
1	A	372	LYS
2	B	1012	PRO
1	A	10	GLU
1	A	125	GLY

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Mol	Chain	Res	Type
1	A	141	PRO
2	B	1010	GLN
1	A	11	GLU
1	A	48	GLU
1	A	116	ALA
1	A	367	ALA
1	A	374	PHE
1	A	210	GLN
1	A	368	ASP
1	A	378	HIS
1	A	394	TYR
1	A	5	ASP
1	A	92	ALA
1	A	136	ASN
1	A	420	ILE
1	A	126	LYS
2	B	1011	ARG
2	B	1006	PRO
1	A	219	PRO
1	A	98	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	A	396/397 (100%)	352 (89%)	44 (11%)	7	28
2	B	12/19 (63%)	7 (58%)	5 (42%)	0	0
All	All	408/416 (98%)	359 (88%)	49 (12%)	6	25

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	ASP
1	A	9	VAL

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Mol	Chain	Res	Type
1	A	18	LYS
1	A	20	LYS
1	A	42	LYS
1	A	48	GLU
1	A	53	ASP
1	A	84	ARG
1	A	88	VAL
1	A	115	THR
1	A	123	LEU
1	A	135	GLU
1	A	138	THR
1	A	144	GLU
1	A	147	LEU
1	A	149	LEU
1	A	202	GLN
1	A	205	SER
1	A	211	ILE
1	A	223	TRP
1	A	224	GLN
1	A	225	ARG
1	A	240	ASP
1	A	274	ILE
1	A	287	ASN
1	A	290	ILE
1	A	301	SER
1	A	311	ASN
1	A	324	GLU
1	A	326	VAL
1	A	329	ASP
1	A	365	THR
1	A	369	LYS
1	A	371	ASP
1	A	378	HIS
1	A	380	ILE
1	A	384	THR
1	A	407	THR
1	A	416	ARG
1	A	437	ASP
1	A	456	ARG
1	A	461	ARG
1	A	467	CYS
2	B	1003	TYR

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Mol	Chain	Res	Type
2	B	1009	ARG
2	B	1010	GLN
2	B	1013	LEU
2	B	1014	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	160	GLN
1	A	188	HIS
1	A	202	GLN
1	A	280	ASN
1	A	307	ASN
1	A	311	ASN
1	A	356	HIS
1	A	362	GLN
1	A	433	HIS
2	B	1010	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

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

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.