



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:58 PM GMT

PDB ID : 1ZBE
Title : Foot-and Mouth Disease Virus Serotype A1061
Authors : Fry, E.E.; Newman, J.W.; Curry, S.; Najjam, S.; Jackson, T.; Blakemore, W.;
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Deposited on : 2005-04-08
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

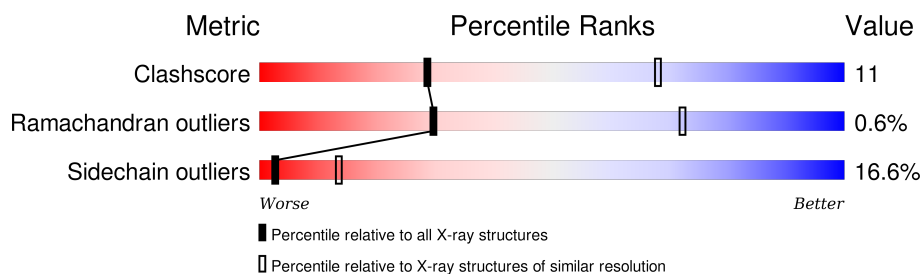
1 Overall quality at a glance

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (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 ≥ 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	212	 68% 16% 6% 10%
2	2	218	 64% 24% 6% • 5%
3	3	221	 66% 30% 5%
4	4	85	 46% 11% • 42%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5227 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 Coat protein VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	191	Total	C	N	O	S	0	0	0
			1492	944	266	278	4			

- Molecule 2 is a protein called Coat protein VP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	207	Total	C	N	O	S	0	0	0
			1652	1061	280	306	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	14	LEU	ILE	ENGINEERED	UNP P03306

- Molecule 3 is a protein called Coat protein VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	221	Total	C	N	O	S	0	0	0
			1708	1089	277	335	7			

- Molecule 4 is a protein called Coat protein VP4.

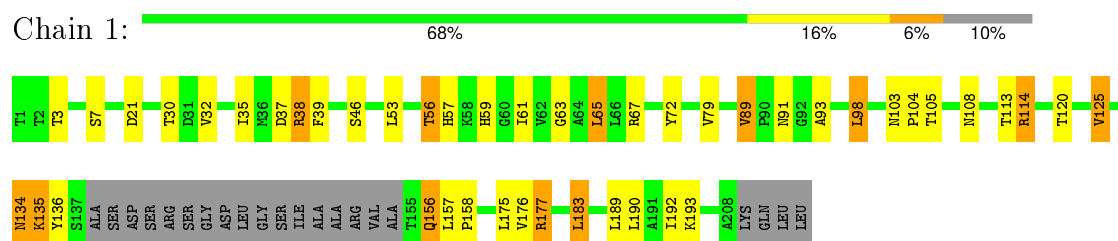
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	49	Total	C	N	O	S	0	0	0
			375	235	62	76	2			

3 Residue-property plots [i](#)

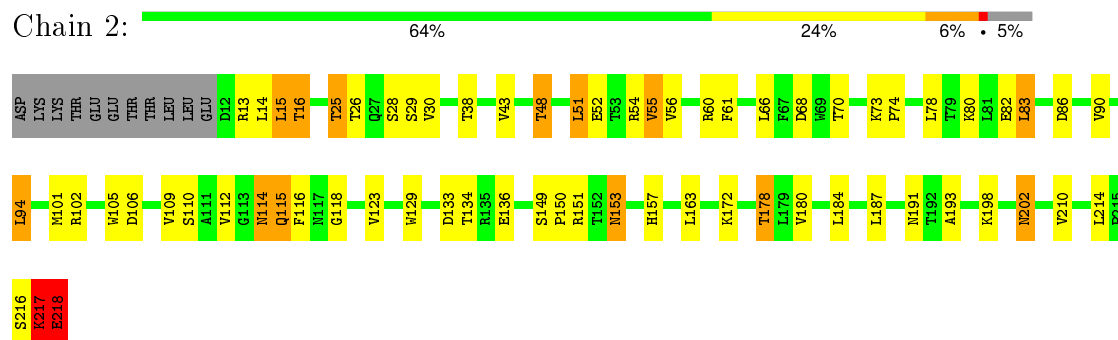
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

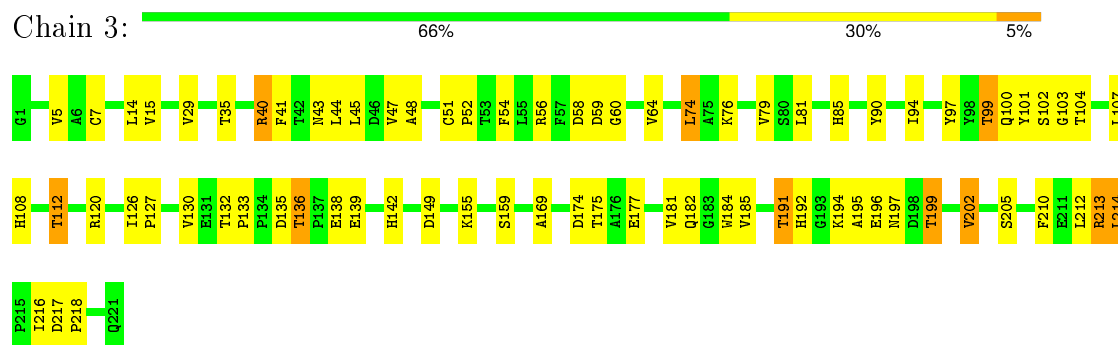
• Molecule 1: Coat protein VP1



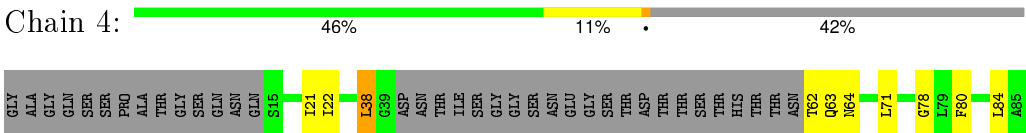
• Molecule 2: Coat protein VP2



• Molecule 3: Coat protein VP3



• Molecule 4: Coat protein VP4



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	306.20 Å 306.20 Å 712.80 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (55.00-3.00)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5227	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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	1	0.54	0/1527	0.83	0/2083
2	2	0.71	2/1701 (0.1%)	0.93	7/2322 (0.3%)
3	3	0.59	1/1757 (0.1%)	0.83	1/2405 (0.0%)
4	4	0.65	0/381	0.90	1/513 (0.2%)
All	All	0.62	3/5366 (0.1%)	0.87	9/7323 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	109	VAL	C-N	13.50	1.65	1.34
2	2	218	GLU	C-O	8.87	1.40	1.23
3	3	51	CYS	CB-SG	-5.68	1.72	1.81

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	218	GLU	CA-C-O	-11.83	95.26	120.10
2	2	217	LYS	O-C-N	10.98	140.27	122.70
2	2	110	SER	O-C-N	6.74	133.48	122.70
2	2	110	SER	CA-C-N	-6.16	103.66	117.20
2	2	217	LYS	CA-C-N	-6.11	103.76	117.20
4	4	38	LEU	CA-CB-CG	5.51	127.97	115.30
2	2	110	SER	C-N-CA	-5.37	108.27	121.70
3	3	54	PHE	N-CA-C	5.22	125.08	111.00
2	2	51	LEU	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1492	0	1485	38	0
2	2	1652	0	1607	36	0
3	3	1708	0	1631	49	0
4	4	375	0	348	3	0
All	All	5227	0	5071	118	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 11.

All (118) 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)
1:1:56:THR:HG22	1:1:67:ARG:HH21	1.24	1.02
3:3:99:THR:HG22	3:3:100:GLN:HG3	1.46	0.95
1:1:56:THR:HG22	1:1:67:ARG:NH2	1.86	0.91
2:2:26:THR:HG22	2:2:28:SER:H	1.39	0.88
1:1:135:LYS:NZ	1:1:158:PRO:HA	1.90	0.87
1:1:57:HIS:HD2	1:1:59:HIS:H	1.23	0.86
2:2:129:TRP:HB2	2:2:178:THR:HG21	1.58	0.86
2:2:115:GLN:H	2:2:115:GLN:HE21	1.21	0.83
3:3:112:THR:HB	3:3:199:THR:HG22	1.60	0.81
3:3:136:THR:HG22	3:3:139:GLU:H	1.51	0.76
1:1:53:LEU:O	1:1:56:THR:HB	1.86	0.76
3:3:99:THR:CG2	3:3:100:GLN:HG3	2.17	0.74
1:1:57:HIS:CD2	1:1:59:HIS:H	2.07	0.72
2:2:216:SER:HB2	3:3:142:HIS:CD2	2.26	0.71
2:2:115:GLN:NE2	2:2:115:GLN:H	1.90	0.70
1:1:135:LYS:HZ2	1:1:158:PRO:HA	1.57	0.69
1:1:91:ASN:O	3:3:99:THR:HG21	1.93	0.67
2:2:106:ASP:OD2	2:2:157:HIS:HE1	1.77	0.67
1:1:103:ASN:HD21	3:3:217:ASP:H	1.42	0.66
3:3:213:ARG:HD3	3:3:214:LEU:HD22	1.78	0.64
3:3:112:THR:CB	3:3:199:THR:HG22	2.28	0.64
2:2:129:TRP:HB2	2:2:178:THR:CG2	2.27	0.64
2:2:16:THR:HB	2:2:25:THR:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:135:LYS:HZ3	1:1:158:PRO:HA	1.61	0.63
1:1:135:LYS:HG3	1:1:158:PRO:HG3	1.81	0.63
2:2:217:LYS:C	2:2:218:GLU:O	2.37	0.62
3:3:191:THR:HG22	3:3:192:HIS:H	1.64	0.62
2:2:115:GLN:N	2:2:115:GLN:HE21	1.94	0.62
1:1:56:THR:HG21	1:1:63:GLY:HA2	1.82	0.62
2:2:133:ASP:HB3	2:2:136:GLU:HG3	1.82	0.61
4:4:38:LEU:O	4:4:38:LEU:HD12	2.01	0.61
3:3:108:HIS:HE1	3:3:205:SER:OG	1.84	0.60
3:3:136:THR:HG22	3:3:139:GLU:HG3	1.83	0.59
2:2:82:GLU:HA	2:2:178:THR:HB	1.84	0.59
4:4:21:ILE:HG22	4:4:22:ILE:HD12	1.86	0.58
1:1:7:SER:HB3	2:2:30:VAL:HG12	1.85	0.57
2:2:218:GLU:HA	2:2:218:GLU:OE1	2.05	0.57
1:1:156:GLN:HE21	1:1:156:GLN:HA	1.70	0.56
3:3:104:THR:CG2	3:3:159:SER:HB3	2.36	0.56
3:3:90:TYR:CE1	3:3:94:ILE:HD11	2.41	0.56
3:3:40:ARG:HG3	3:3:41:PHE:N	2.21	0.56
1:1:89:VAL:HG13	1:1:93:ALA:HB3	1.87	0.55
1:1:91:ASN:CB	1:1:120:THR:HG23	2.36	0.55
3:3:64:VAL:CG1	3:3:74:LEU:HG	2.37	0.55
2:2:61:PHE:HB3	2:2:202:ASN:HD21	1.72	0.55
1:1:134:ASN:O	1:1:135:LYS:HB3	2.06	0.54
3:3:192:HIS:HB2	3:3:195:ALA:HB3	1.90	0.54
1:1:91:ASN:HB3	1:1:120:THR:HG23	1.91	0.53
2:2:216:SER:HB2	3:3:142:HIS:HD2	1.74	0.52
1:1:89:VAL:HG22	3:3:216:ILE:HD11	1.92	0.52
3:3:136:THR:CG2	3:3:139:GLU:HG3	2.40	0.52
2:2:114:ASN:HD21	2:2:193:ALA:HA	1.74	0.52
3:3:133:PRO:HG3	3:3:184:TRP:CD2	2.45	0.51
3:3:85:HIS:H	3:3:85:HIS:CD2	2.26	0.51
1:1:37:ASP:OD2	1:1:177:ARG:HD3	2.11	0.51
1:1:79:VAL:HG22	1:1:114:ARG:HG3	1.91	0.51
1:1:35:ILE:O	1:1:38:ARG:HD2	2.09	0.50
3:3:79:VAL:HG22	3:3:185:VAL:HG23	1.93	0.50
3:3:56:ARG:NH1	3:3:56:ARG:HG2	2.25	0.50
3:3:108:HIS:O	3:3:202:VAL:HA	2.12	0.49
3:3:97:TYR:C	3:3:216:ILE:HG22	2.33	0.49
3:3:56:ARG:HG2	3:3:56:ARG:HH11	1.77	0.49
1:1:89:VAL:HB	1:1:98:LEU:CD1	2.42	0.49
3:3:43:ASN:HD22	3:3:45:LEU:H	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:135:LYS:O	1:1:135:LYS:HG2	2.14	0.48
3:3:120:ARG:NH1	3:3:149:ASP:HB3	2.29	0.48
3:3:120:ARG:HH11	3:3:149:ASP:HB3	1.78	0.47
2:2:114:ASN:HD22	2:2:114:ASN:C	2.17	0.47
2:2:55:VAL:HG22	2:2:55:VAL:O	2.14	0.47
2:2:15:LEU:HD22	2:2:16:THR:N	2.30	0.47
3:3:47:VAL:HG22	3:3:90:TYR:CE1	2.50	0.47
1:1:89:VAL:CG1	1:1:93:ALA:HB3	2.45	0.47
1:1:32:VAL:HG13	1:1:183:LEU:HD22	1.96	0.47
2:2:153:ASN:N	2:2:153:ASN:HD22	2.13	0.47
2:2:83:LEU:HB3	2:2:105:TRP:CZ2	2.49	0.46
1:1:39:PHE:CE1	1:1:177:ARG:HB2	2.51	0.46
3:3:181:VAL:HG12	3:3:182:GLN:NE2	2.30	0.46
2:2:214:LEU:HD23	3:3:127:PRO:HG2	1.97	0.46
2:2:48:THR:HG21	2:2:52:GLU:HB3	1.98	0.45
3:3:45:LEU:HA	3:3:48:ALA:HB3	1.99	0.45
2:2:94:LEU:HG	2:2:210:VAL:HG11	1.98	0.45
2:2:149:SER:H	2:2:153:ASN:ND2	2.15	0.45
2:2:43:VAL:HG12	2:2:102:ARG:NE	2.31	0.45
2:2:184:LEU:HA	2:2:184:LEU:HD12	1.75	0.45
1:1:56:THR:CG2	1:1:67:ARG:HH21	2.11	0.45
2:2:101:MET:HG2	2:2:210:VAL:HG12	1.99	0.45
3:3:213:ARG:O	3:3:214:LEU:HB2	2.17	0.44
1:1:72:TYR:O	1:1:125:VAL:HG22	2.18	0.44
2:2:78:LEU:HD23	2:2:78:LEU:C	2.38	0.44
3:3:174:ASP:O	3:3:177:GLU:HB2	2.18	0.44
3:3:196:GLU:O	3:3:197:ASN:HB2	2.16	0.44
3:3:43:ASN:ND2	3:3:45:LEU:H	2.16	0.43
1:1:56:THR:O	1:1:67:ARG:NH2	2.51	0.43
3:3:103:GLY:HA3	3:3:210:PHE:HA	2.00	0.43
1:1:79:VAL:HB	1:1:175:LEU:HB2	2.01	0.43
1:1:65:LEU:HD12	1:1:65:LEU:HA	1.81	0.43
3:3:126:ILE:N	3:3:126:ILE:HD12	2.34	0.43
3:3:52:PRO:HB3	3:3:205:SER:HB3	2.01	0.42
2:2:114:ASN:ND2	2:2:116:PHE:H	2.17	0.42
2:2:68:ASP:OD1	2:2:198:LYS:HG2	2.19	0.42
1:1:183:LEU:HD12	1:1:183:LEU:HA	1.79	0.42
2:2:218:GLU:OE1	2:2:218:GLU:CA	2.68	0.42
3:3:14:LEU:HD12	3:3:15:VAL:N	2.35	0.42
1:1:61:ILE:O	1:1:65:LEU:HB2	2.20	0.41
1:1:79:VAL:CG2	1:1:114:ARG:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:105:THR:O	3:3:15:VAL:HA	2.19	0.41
3:3:104:THR:HG21	3:3:159:SER:HB3	2.01	0.41
2:2:118:GLY:O	2:2:187:LEU:HD12	2.19	0.41
1:1:56:THR:CG2	1:1:63:GLY:HA2	2.50	0.41
3:3:74:LEU:HD12	3:3:74:LEU:HA	1.86	0.41
3:3:101:TYR:CD2	3:3:102:SER:N	2.89	0.41
3:3:100:GLN:HA	3:3:169:ALA:O	2.20	0.41
4:4:71:LEU:HA	4:4:71:LEU:HD12	1.88	0.40
3:3:136:THR:HG23	3:3:138:GLU:H	1.87	0.40
2:2:216:SER:OG	2:2:218:GLU:OE1	2.35	0.40
2:2:114:ASN:ND2	2:2:114:ASN:C	2.75	0.40
1:1:79:VAL:HA	1:1:113:THR:O	2.22	0.40
3:3:181:VAL:HG12	3:3:182:GLN:HE21	1.87	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	187/212 (88%)	174 (93%)	12 (6%)	1 (0%)	34	76
2	2	205/218 (94%)	192 (94%)	13 (6%)	0	100	100
3	3	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	21	64
4	4	45/85 (53%)	40 (89%)	4 (9%)	1 (2%)	8	38
All	All	656/736 (89%)	613 (93%)	39 (6%)	4 (1%)	30	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	78	GLY
3	3	60	GLY

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Mol	Chain	Res	Type
1	1	104	PRO
3	3	218	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	161/176 (92%)	137 (85%)	24 (15%)	4	17
2	2	181/192 (94%)	143 (79%)	38 (21%)	1	7
3	3	183/183 (100%)	156 (85%)	27 (15%)	4	17
4	4	40/68 (59%)	35 (88%)	5 (12%)	6	24
All	All	565/619 (91%)	471 (83%)	94 (17%)	3	13

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	3	THR
1	1	21	ASP
1	1	30	THR
1	1	38	ARG
1	1	46	SER
1	1	56	THR
1	1	65	LEU
1	1	89	VAL
1	1	98	LEU
1	1	108	ASN
1	1	114	ARG
1	1	125	VAL
1	1	134	ASN
1	1	135	LYS
1	1	136	TYR
1	1	156	GLN
1	1	157	LEU
1	1	176	VAL
1	1	177	ARG

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Mol	Chain	Res	Type
1	1	183	LEU
1	1	189	LEU
1	1	190	LEU
1	1	192	ILE
1	1	193	LYS
2	2	13	ARG
2	2	14	LEU
2	2	15	LEU
2	2	16	THR
2	2	25	THR
2	2	29	SER
2	2	38	THR
2	2	48	THR
2	2	51	LEU
2	2	54	ARG
2	2	55	VAL
2	2	56	VAL
2	2	60	ARG
2	2	66	LEU
2	2	70	THR
2	2	73	LYS
2	2	74	PRO
2	2	80	LYS
2	2	83	LEU
2	2	86	ASP
2	2	90	VAL
2	2	94	LEU
2	2	112	VAL
2	2	114	ASN
2	2	115	GLN
2	2	123	VAL
2	2	134	THR
2	2	150	PRO
2	2	151	ARG
2	2	153	ASN
2	2	163	LEU
2	2	172	LYS
2	2	178	THR
2	2	180	VAL
2	2	191	ASN
2	2	202	ASN
2	2	217	LYS

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Mol	Chain	Res	Type
2	2	218	GLU
3	3	5	VAL
3	3	7	CYS
3	3	29	VAL
3	3	35	THR
3	3	40	ARG
3	3	44	LEU
3	3	58	ASP
3	3	59	ASP
3	3	74	LEU
3	3	76	LYS
3	3	81	LEU
3	3	99	THR
3	3	107	LEU
3	3	112	THR
3	3	130	VAL
3	3	132	THR
3	3	135	ASP
3	3	136	THR
3	3	155	LYS
3	3	175	THR
3	3	191	THR
3	3	194	LYS
3	3	199	THR
3	3	202	VAL
3	3	212	LEU
3	3	213	ARG
3	3	214	LEU
4	4	62	THR
4	4	63	GLN
4	4	64	ASN
4	4	80	PHE
4	4	84	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	57	HIS
1	1	103	ASN
1	1	108	ASN
1	1	156	GLN
1	1	167	GLN

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Mol	Chain	Res	Type
1	1	169	GLN
2	2	114	ASN
2	2	115	GLN
2	2	153	ASN
2	2	157	HIS
2	2	202	ASN
3	3	36	ASN
3	3	43	ASN
3	3	85	HIS
3	3	108	HIS
3	3	142	HIS
3	3	153	ASN
3	3	180	ASN
4	4	17	ASN
4	4	64	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.