Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 08:26 AM EST

PDB ID	:	1FOD
Title	:	STRUCTURE OF A MAJOR IMMUNOGENIC SITE ON FOOT-AND-MOUTH DISEASE VIRUS
Authors	:	Logan, D.T.; Lea, S.; Lewis, R.; Stuart, D.; Fry, E.
Deposited on	:	1993-10-27
Resolution	:	2.60 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

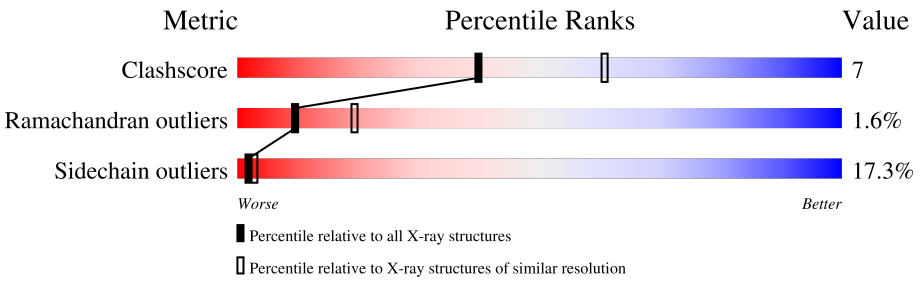
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	213	65% 20% 11% • •
2	2	218	64% 22% 9% • •
3	3	220	70% 20% 7% •
4	4	85	38% 13% • • 45%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5362 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	210	1651	1041	299	306	5	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	56	VAL	ILE	conflict	UNP Q84771
1	64	GLY	ALA	conflict	UNP Q84771
1	137	SER	ASN	conflict	UNP Q84771

- Molecule 2 is a protein called FOOT AND MOUTH DISEASE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	2	214	1676	1065	286	318	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	130	CYS	TYR	conflict	UNP Q84771

- Molecule 3 is a protein called FOOT AND MOUTH DISEASE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	3	220	1681	1075	275	322	9	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	85	HIS	GLN	conflict	UNP Q84771

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Chain	Residue	Modelled	Actual	Comment	Reference
3	168	THR	ALA	conflict	UNP Q84771
3	173	ASP	GLY	conflict	UNP Q84771

- Molecule 4 is a protein called FOOT AND MOUTH DISEASE VIRUS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	4	47	354	222	58	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. 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. 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.

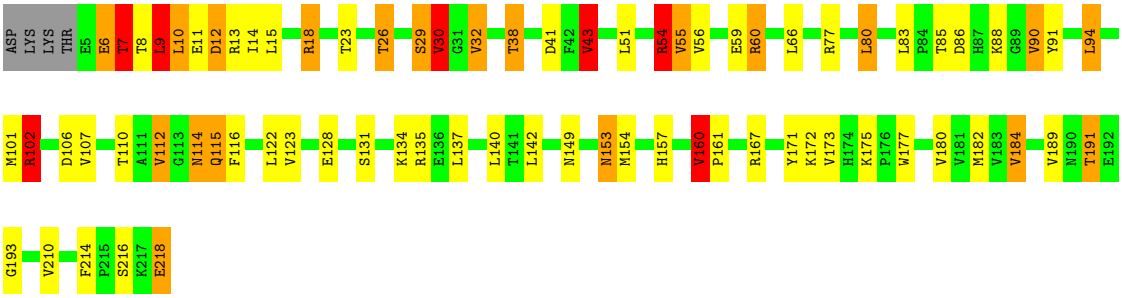
Note EDS was not executed.

• Molecule 1: FOOT AND MOUTH DISEASE VIRUS

Chain 1:

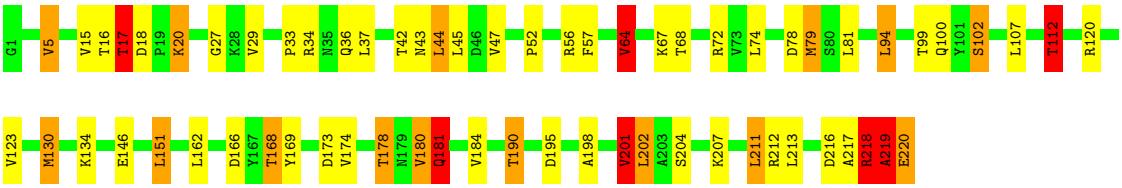
• Molecule 2: FOOT AND MOUTH DISEASE VIRUS

Chain 2:



• Molecule 3: FOOT AND MOUTH DISEASE VIRUS

Chain 3:



• Molecule 4: FOOT AND MOUTH DISEASE VIRUS

Chain 4:

GLY
ALA
GLY
GLN
SER
SER
PRO
ALA
THR
GLY
SER
GLN
ASN
GLN
S15
I22
N23
Y26
M27
Q28
Q29
Y30
M34
D35
D40
ASN
ALA
ILE
SER
GLY
GLY
SER
ASN
GLU
GLY
SER
THR
ASP
THR
THR
SER
THR
HIS
THR
THR
ASN
THR
GLN
ASN
N65
D66
S69
L79
F80

G81
A82
A85

4 Data and refinement statistics (i)

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, α, β, γ	345.00Å 345.00Å 345.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5362	wwPDB-VP
Average B, all atoms ($Å^2$)	15.0	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	1.12	1/1688 (0.1%)	1.96	43/2303 (1.9%)
2	2	1.16	6/1719 (0.3%)	1.88	41/2346 (1.7%)
3	3	1.10	3/1729 (0.2%)	1.89	47/2361 (2.0%)
4	4	1.10	1/360 (0.3%)	1.96	11/483 (2.3%)
All	All	1.12	11/5496 (0.2%)	1.91	142/7493 (1.9%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	167	ARG	CZ-NH2	6.94	1.42	1.33
4	4	69	SER	CA-CB	-6.81	1.42	1.52
2	2	112	VAL	CA-CB	6.39	1.68	1.54
2	2	32	VAL	CA-CB	6.30	1.68	1.54
2	2	14	ILE	CA-CB	6.10	1.68	1.54
1	1	173	VAL	CA-CB	5.98	1.67	1.54
2	2	55	VAL	CA-CB	5.71	1.66	1.54
3	3	29	VAL	CA-CB	5.57	1.66	1.54
2	2	184	VAL	CA-CB	5.31	1.65	1.54
3	3	47	VAL	CA-CB	5.27	1.65	1.54
3	3	218	ARG	CZ-NH2	5.11	1.39	1.33

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	135	ARG	NE-CZ-NH1	21.32	130.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	135	ARG	NE-CZ-NH2	-15.58	112.51	120.30
3	3	72	ARG	NE-CZ-NH2	-14.38	113.11	120.30
1	1	182	ARG	NE-CZ-NH1	13.34	126.97	120.30
2	2	18	ARG	NE-CZ-NH2	-13.34	113.63	120.30
3	3	34	ARG	NE-CZ-NH1	13.19	126.90	120.30
1	1	179	ARG	NE-CZ-NH1	13.05	126.82	120.30
1	1	182	ARG	NE-CZ-NH2	-12.79	113.91	120.30
1	1	179	ARG	NE-CZ-NH2	-11.83	114.39	120.30
1	1	136	TYR	CB-CG-CD2	-11.36	114.19	121.00
1	1	145	ARG	NE-CZ-NH2	-11.30	114.65	120.30
3	3	218	ARG	NE-CZ-NH1	-11.02	114.79	120.30
1	1	208	PRO	CA-C-N	-10.49	94.13	117.20
2	2	7	THR	N-CA-C	10.06	138.16	111.00
1	1	200	ARG	NE-CZ-NH2	-9.81	115.40	120.30
3	3	42	THR	CA-CB-CG2	9.65	125.91	112.40
1	1	208	PRO	O-C-N	9.63	138.12	122.70
2	2	13	ARG	NE-CZ-NH2	-9.58	115.51	120.30
3	3	219	ALA	N-CA-C	9.51	136.67	111.00
2	2	54	ARG	NE-CZ-NH2	9.45	125.03	120.30
3	3	123	VAL	CG1-CB-CG2	9.45	126.02	110.90
3	3	218	ARG	CA-CB-CG	9.20	133.64	113.40
3	3	180	VAL	CA-C-N	-9.10	97.19	117.20
1	1	114	ARG	NE-CZ-NH1	8.91	124.76	120.30
3	3	218	ARG	N-CA-C	-8.77	87.32	111.00
3	3	102	SER	CA-CB-OG	-8.68	87.76	111.20
3	3	202	LEU	CA-CB-CG	8.65	135.20	115.30
4	4	30	TYR	CB-CG-CD2	-8.52	115.89	121.00
2	2	102	ARG	NE-CZ-NH1	8.29	124.45	120.30
3	3	130	MET	CA-CB-CG	8.18	127.21	113.30
1	1	200	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	1	147	ASP	CB-CG-OD2	-8.13	110.98	118.30
3	3	17	THR	N-CA-CB	-8.06	94.98	110.30
3	3	72	ARG	NE-CZ-NH1	7.99	124.30	120.30
4	4	35	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	1	200	ARG	CD-NE-CZ	7.95	134.73	123.60
2	2	102	ARG	NE-CZ-NH2	-7.86	116.37	120.30
3	3	42	THR	CA-CB-OG1	-7.75	92.73	109.00
3	3	168	THR	CA-CB-CG2	-7.74	101.57	112.40
1	1	136	TYR	CB-CG-CD1	7.65	125.59	121.00
2	2	60	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	1	101	THR	CA-CB-CG2	7.61	123.05	112.40
1	1	96	LYS	CA-CB-CG	7.59	130.09	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	124	ARG	NE-CZ-NH1	7.57	124.08	120.30
2	2	13	ARG	N-CA-C	-7.44	90.92	111.00
2	2	218	GLU	CA-CB-CG	7.40	129.69	113.40
1	1	182	ARG	CA-CB-CG	7.35	129.57	113.40
2	2	30	VAL	CA-CB-CG2	-7.33	99.91	110.90
2	2	30	VAL	CA-CB-CG1	7.26	121.78	110.90
2	2	7	THR	CA-CB-CG2	-7.19	102.34	112.40
1	1	101	THR	N-CA-CB	-7.16	96.70	110.30
3	3	220	GLU	CA-CB-CG	7.16	129.14	113.40
3	3	64	VAL	N-CA-CB	-7.07	95.94	111.50
4	4	65	ASN	CA-C-O	-7.05	105.29	120.10
2	2	6	GLU	N-CA-C	6.97	129.82	111.00
2	2	172	LYS	CB-CG-CD	6.96	129.69	111.60
1	1	129	VAL	CA-CB-CG2	-6.95	100.48	110.90
1	1	114	ARG	CA-CB-CG	6.91	128.59	113.40
3	3	180	VAL	CA-C-O	6.86	134.50	120.10
1	1	50	ILE	CB-CG1-CD1	-6.85	94.71	113.90
1	1	114	ARG	NE-CZ-NH2	-6.85	116.88	120.30
3	3	36	GLN	CA-CB-CG	-6.83	98.37	113.40
3	3	68	THR	OG1-CB-CG2	6.82	125.69	110.00
1	1	182	ARG	CD-NE-CZ	6.81	133.13	123.60
4	4	35	ASP	CB-CG-OD1	6.77	124.39	118.30
3	3	217	ALA	C-N-CA	6.73	138.52	121.70
4	4	65	ASN	N-CA-CB	6.69	122.64	110.60
2	2	9	LEU	CA-CB-CG	6.60	130.49	115.30
4	4	30	TYR	CB-CG-CD1	6.60	124.96	121.00
2	2	43	VAL	N-CA-CB	-6.59	97.01	111.50
1	1	89	VAL	N-CA-CB	-6.58	97.02	111.50
3	3	56	ARG	NE-CZ-NH1	6.53	123.57	120.30
2	2	29	SER	CA-C-N	6.52	131.55	117.20
2	2	10	LEU	CA-C-N	6.50	131.51	117.20
3	3	20	LYS	N-CA-CB	-6.48	98.94	110.60
2	2	26	THR	N-CA-CB	6.47	122.60	110.30
1	1	115	LEU	CB-CG-CD2	-6.42	100.09	111.00
2	2	135	ARG	CD-NE-CZ	6.41	132.57	123.60
1	1	172	ARG	CA-CB-CG	6.39	127.45	113.40
2	2	123	VAL	CG1-CB-CG2	6.38	121.11	110.90
2	2	18	ARG	CA-CB-CG	-6.37	99.38	113.40
3	3	211	LEU	CA-CB-CG	6.34	129.89	115.30
3	3	27	GLY	CA-C-N	-6.32	103.30	117.20
1	1	26	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	2	182	MET	CG-SD-CE	6.17	110.08	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	78	ASP	CB-CG-OD1	6.12	123.81	118.30
3	3	34	ARG	NH1-CZ-NH2	-6.10	112.69	119.40
2	2	6	GLU	C-N-CA	6.10	136.94	121.70
3	3	112	THR	N-CA-CB	-6.09	98.73	110.30
4	4	65	ASN	CA-C-N	6.04	130.49	117.20
4	4	26	TYR	CB-CG-CD2	6.04	124.62	121.00
2	2	26	THR	CB-CA-C	-6.03	95.31	111.60
4	4	34	MET	CA-CB-CG	6.03	123.55	113.30
2	2	167	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	1	147	ASP	CA-CB-CG	5.97	126.55	113.40
1	1	114	ARG	CD-NE-CZ	5.86	131.80	123.60
4	4	27	MET	CA-CB-CG	-5.85	103.36	113.30
3	3	169	TYR	CB-CG-CD1	5.83	124.50	121.00
3	3	173	ASP	O-C-N	5.80	131.98	122.70
3	3	64	VAL	CB-CA-C	5.77	122.36	111.40
1	1	206	VAL	N-CA-CB	-5.76	98.83	111.50
2	2	18	ARG	NH1-CZ-NH2	5.76	125.74	119.40
1	1	137	SER	CA-C-N	-5.76	104.53	117.20
2	2	80	LEU	CA-CB-CG	5.71	128.42	115.30
1	1	120	THR	CA-C-N	5.69	129.71	117.20
1	1	209	VAL	CA-CB-CG2	-5.66	102.41	110.90
2	2	160	VAL	N-CA-CB	-5.63	99.12	111.50
3	3	181	GLN	CA-CB-CG	5.63	125.78	113.40
3	3	178	THR	CA-CB-CG2	-5.62	104.53	112.40
3	3	166	ASP	CB-CG-OD1	5.60	123.34	118.30
1	1	125	VAL	N-CA-CB	-5.60	99.18	111.50
3	3	34	ARG	CG-CD-NE	-5.54	100.16	111.80
2	2	171	TYR	CB-CG-CD2	-5.52	117.69	121.00
3	3	190	THR	N-CA-CB	5.52	120.78	110.30
2	2	191	THR	OG1-CB-CG2	-5.51	97.32	110.00
2	2	38	THR	CA-CB-CG2	5.51	120.12	112.40
3	3	201	VAL	CG1-CB-CG2	5.46	119.64	110.90
1	1	178	TYR	CB-CG-CD2	5.46	124.28	121.00
3	3	33	PRO	N-CD-CG	-5.45	95.02	103.20
1	1	101	THR	CA-CB-OG1	-5.43	97.60	109.00
1	1	159	LEU	CB-CG-CD2	-5.40	101.82	111.00
3	3	151	LEU	CB-CG-CD1	-5.40	101.82	111.00
3	3	68	THR	CA-C-N	-5.39	105.33	117.20
3	3	217	ALA	N-CA-CB	-5.39	102.55	110.10
2	2	12	ASP	CA-CB-CG	5.38	125.24	113.40
3	3	20	LYS	CB-CA-C	5.37	121.14	110.40
3	3	5	VAL	CA-CB-CG2	-5.36	102.86	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	88	LYS	CA-CB-CG	5.30	125.06	113.40
1	1	208	PRO	CA-N-CD	-5.30	104.08	111.50
1	1	56	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	1	72	TYR	CB-CG-CD2	5.26	124.15	121.00
1	1	89	VAL	CB-CA-C	5.25	121.38	111.40
2	2	173	VAL	CA-CB-CG1	-5.21	103.09	110.90
2	2	14	ILE	CB-CA-C	-5.20	101.20	111.60
3	3	219	ALA	CA-C-N	5.12	128.46	117.20
4	4	82	ALA	N-CA-C	-5.11	97.20	111.00
2	2	90	VAL	CA-CB-CG2	5.10	118.55	110.90
2	2	41	ASP	CB-CG-OD1	5.07	122.86	118.30
3	3	218	ARG	CD-NE-CZ	5.06	130.68	123.60
1	1	38	ARG	CA-CB-CG	5.05	124.52	113.40
2	2	7	THR	CA-CB-OG1	5.01	119.52	109.00
3	3	64	VAL	CG1-CB-CG2	5.01	118.92	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	3	16	THR	Mainchain

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	1651	0	1670	30	0
2	2	1676	0	1625	30	0
3	3	1681	0	1616	23	0
4	4	354	0	324	6	0
All	All	5362	0	5235	77	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 7.

All (77) 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)
1:1:1:THR:HG23	4:4:79:LEU:HA	1.46	0.94
3:3:100:GLN:HE22	3:3:212:ARG:HH21	1.15	0.94
4:4:65:ASN:HA	4:4:69:SER:HB2	1.51	0.93
2:2:114:ASN:HD21	2:2:193:GLY:HA2	1.42	0.82
2:2:115:GLN:HE21	2:2:115:GLN:H	1.28	0.82
3:3:100:GLN:NE2	3:3:212:ARG:HH21	1.85	0.74
3:3:43:ASN:HD22	3:3:45:LEU:H	1.34	0.74
1:1:7:SER:O	1:1:8:ALA:HB3	1.87	0.73
1:1:1:THR:HG23	4:4:79:LEU:CA	2.19	0.73
2:2:18:ARG:HG3	2:2:23:THR:HG22	1.70	0.73
1:1:103:ASN:HD21	3:3:216:ASP:H	1.35	0.72
2:2:6:GLU:HB3	2:2:12:ASP:HB3	1.71	0.72
4:4:65:ASN:CA	4:4:69:SER:HB2	2.20	0.72
1:1:35:ILE:O	1:1:38:ARG:HD2	1.90	0.71
1:1:144:LEU:HG	1:1:150:VAL:HG13	1.76	0.68
3:3:100:GLN:HE22	3:3:212:ARG:NH2	1.91	0.67
2:2:115:GLN:H	2:2:115:GLN:NE2	1.93	0.65
3:3:64:VAL:HG13	3:3:74:LEU:HG	1.80	0.63
3:3:168:THR:HG21	3:3:181:GLN:NE2	2.14	0.62
1:1:98:LEU:HG	1:1:169:LYS:HB2	1.83	0.61
1:1:134:CYS:SG	1:1:161:THR:HG23	2.42	0.59
3:3:52:PRO:HB3	3:3:204:SER:HB3	1.83	0.59
1:1:7:SER:O	1:1:8:ALA:CB	2.48	0.59
2:2:106:ASP:OD1	2:2:157:HIS:HE1	1.85	0.59
1:1:25:GLN:HG2	1:1:27:ARG:HG3	1.86	0.58
1:1:151:LEU:HD13	2:2:131:SER:HA	1.87	0.57
2:2:114:ASN:ND2	2:2:193:GLY:HA2	2.19	0.55
3:3:64:VAL:CG1	3:3:74:LEU:HG	2.36	0.55
1:1:89:VAL:HB	1:1:98:LEU:HD13	1.88	0.55
1:1:45:GLN:H	1:1:49:ASN:HD21	1.53	0.55
1:1:141:VAL:HG12	2:2:175:LYS:NZ	2.22	0.55
1:1:104:PRO:HG3	3:3:17:THR:HG21	1.89	0.55
1:1:113:THR:HG22	1:1:115:LEU:HD13	1.88	0.54
1:1:141:VAL:HG12	2:2:175:LYS:HZ3	1.73	0.54
2:2:114:ASN:ND2	2:2:116:PHE:H	2.06	0.53
2:2:101:MET:HG2	2:2:210:VAL:HG12	1.92	0.52
3:3:44:LEU:HG	3:3:94:LEU:HD21	1.91	0.52
1:1:89:VAL:HG13	1:1:93:ALA:CB	2.40	0.52
2:2:216:SER:OG	2:2:218:GLU:HG2	2.11	0.52
4:4:65:ASN:HA	4:4:69:SER:CB	2.32	0.51
1:1:103:ASN:ND2	3:3:216:ASP:H	2.07	0.51
3:3:79:MET:CE	3:3:79:MET:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:79:MET:HA	3:3:79:MET:HE2	1.94	0.49
2:2:107:VAL:O	2:2:157:HIS:HA	2.12	0.48
1:1:61:LEU:O	1:1:65:LEU:HB2	2.14	0.48
1:1:209:VAL:HG12	1:1:210:LYS:HG3	1.95	0.48
1:1:89:VAL:HG13	1:1:93:ALA:HB3	1.95	0.47
1:1:6:GLU:HG2	2:2:153:ASN:ND2	2.29	0.47
3:3:15:VAL:HB	3:3:18:ASP:HB3	1.96	0.47
2:2:149:ASN:H	2:2:153:ASN:ND2	2.14	0.46
2:2:43:VAL:HG22	2:2:102:ARG:HD2	1.97	0.46
2:2:114:ASN:HB2	2:2:115:GLN:HE21	1.81	0.45
1:1:44:PRO:HB2	1:1:173:VAL:HG22	1.97	0.45
3:3:57:PHE:CE2	3:3:201:VAL:HG13	2.52	0.45
1:1:129:VAL:HG13	2:2:128:GLU:HB2	1.99	0.45
2:2:54:ARG:NH1	2:2:59:GLU:OE1	2.50	0.45
2:2:9:LEU:HD12	2:2:10:LEU:HG	1.99	0.44
2:2:115:GLN:HE21	2:2:115:GLN:N	2.04	0.44
1:1:56:VAL:HA	1:1:57:PRO:HD3	1.84	0.44
2:2:214:PHE:CD1	3:3:130:MET:HG2	2.53	0.44
2:2:122:LEU:HD23	2:2:140:LEU:HD23	1.99	0.43
3:3:18:ASP:OD2	3:3:20:LYS:HE2	2.18	0.43
1:1:90:PRO:HG2	3:3:99:THR:HG21	2.00	0.43
3:3:120:ARG:HH11	3:3:146:GLU:HG2	1.83	0.43
2:2:112:VAL:HB	2:2:154:MET:SD	2.58	0.43
1:1:24:ILE:HD11	1:1:26:ARG:HG3	2.01	0.43
3:3:112:THR:HB	3:3:198:ALA:O	2.18	0.43
2:2:91:TYR:O	2:2:94:LEU:HB2	2.19	0.42
2:2:29:SER:O	2:2:30:VAL:HB	2.20	0.42
1:1:37:ASP:OD1	1:1:179:ARG:HD2	2.21	0.41
2:2:134:LYS:O	2:2:137:LEU:HB2	2.21	0.41
3:3:218:ARG:HE	3:3:219:ALA:H	1.68	0.41
4:4:22:ILE:HD12	4:4:23:ASN:O	2.19	0.41
3:3:43:ASN:ND2	3:3:45:LEU:H	2.09	0.41
2:2:142:LEU:HD23	2:2:142:LEU:HA	1.83	0.41
2:2:160:VAL:HG13	2:2:177:TRP:CZ2	2.56	0.40
1:1:142:PRO:HG2	1:1:144:LEU:HD13	2.02	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	208/213 (98%)	197 (95%)	9 (4%)	2 (1%)	15 32
2	2	212/218 (97%)	195 (92%)	13 (6%)	4 (2%)	8 15
3	3	218/220 (99%)	206 (94%)	9 (4%)	3 (1%)	11 22
4	4	43/85 (51%)	37 (86%)	4 (9%)	2 (5%)	2 2
All	All	681/736 (92%)	635 (93%)	35 (5%)	11 (2%)	9 19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	209	VAL
2	2	8	THR
2	2	9	LEU
2	2	30	VAL
3	3	174	VAL
4	4	66	ASP
2	2	7	THR
3	3	219	ALA
1	1	104	PRO
3	3	218	ARG
4	4	81	GLY

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	180/183 (98%)	145 (81%)	35 (19%)	1 2
2	2	185/191 (97%)	153 (83%)	32 (17%)	2 3
3	3	176/176 (100%)	148 (84%)	28 (16%)	2 4
4	4	37/67 (55%)	32 (86%)	5 (14%)	4 6
All	All	578/617 (94%)	478 (83%)	100 (17%)	2 3

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1	THR
1	1	24	ILE
1	1	25	GLN
1	1	38	ARG
1	1	44	PRO
1	1	50	ILE
1	1	53	LEU
1	1	56	VAL
1	1	65	LEU
1	1	89	VAL
1	1	96	LYS
1	1	98	LEU
1	1	111	PRO
1	1	114	ARG
1	1	118	PRO
1	1	124	ARG
1	1	125	VAL
1	1	135	ARG
1	1	136	TYR
1	1	138	ARG
1	1	144	LEU
1	1	148	LEU
1	1	158	THR
1	1	159	LEU
1	1	160	PRO
1	1	172	ARG
1	1	173	VAL
1	1	191	LEU
1	1	192	LEU
1	1	194	ILE
1	1	197	THR
1	1	204	LYS
1	1	206	VAL

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Mol	Chain	Res	Type
1	1	208	PRO
1	1	210	LYS
2	2	7	THR
2	2	9	LEU
2	2	11	GLU
2	2	15	LEU
2	2	26	THR
2	2	32	VAL
2	2	38	THR
2	2	43	VAL
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	77	ARG
2	2	80	LEU
2	2	83	LEU
2	2	85	THR
2	2	86	ASP
2	2	90	VAL
2	2	94	LEU
2	2	102	ARG
2	2	110	THR
2	2	114	ASN
2	2	115	GLN
2	2	153	ASN
2	2	160	VAL
2	2	161	PRO
2	2	180	VAL
2	2	184	VAL
2	2	189	VAL
2	2	191	THR
3	3	5	VAL
3	3	17	THR
3	3	37	LEU
3	3	44	LEU
3	3	64	VAL
3	3	67	LYS
3	3	79	MET
3	3	81	LEU

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Mol	Chain	Res	Type
3	3	94	LEU
3	3	102	SER
3	3	107	LEU
3	3	112	THR
3	3	134	LYS
3	3	151	LEU
3	3	162	LEU
3	3	178	THR
3	3	180	VAL
3	3	181	GLN
3	3	184	VAL
3	3	190	THR
3	3	195	ASP
3	3	201	VAL
3	3	202	LEU
3	3	207	LYS
3	3	211	LEU
3	3	213	LEU
3	3	218	ARG
3	3	220	GLU
4	4	23	ASN
4	4	28	GLN
4	4	66	ASP
4	4	69	SER
4	4	80	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	25	GLN
1	1	49	ASN
1	1	55	GLN
1	1	103	ASN
2	2	114	ASN
2	2	115	GLN
2	2	153	ASN
2	2	157	HIS
2	2	166	ASN
2	2	196	GLN
3	3	43	ASN
3	3	100	GLN
3	3	152	ASN

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Mol	Chain	Res	Type
4	4	31	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 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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.