Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:26 PM GMT

PDB ID	:	1TME
Title	:	THREE-DIMENSIONAL STRUCTURE OF THEILER VIRUS
Authors	:	Grant, R.A.; Filman, D.J.; Hogle, J.M.
Deposited on	:	1992-01-30
Resolution	:	2.80 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 (i) symbol.

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

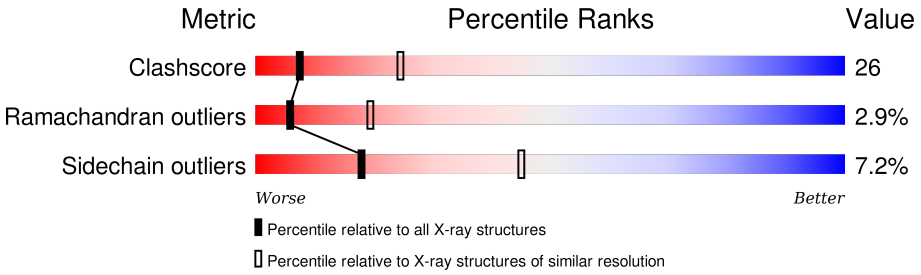
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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 <=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	274	37% 35% 19% • 7%
2	2	267	40% 40% 15% • •
3	3	236	38% 44% 12% • •
4	4	71	10% 17% • • 65%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6280 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 THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	256	Total	C	N	O	S	0	0	0
			2005	1293	335	368	9			

- Molecule 2 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	255	Total	C	N	O	S	0	0	0
			1982	1246	350	378	8			

- Molecule 3 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	230	Total	C	N	O	S	0	0	0
			1774	1139	287	336	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	202	THR	ALA	CONFLICT	UNP P13899
3	230	VAL	ALA	CONFLICT	UNP P13899

- Molecule 4 is a protein called THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP4).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	4	25	Total	C	N	O	0	0	0
			192	117	32	43			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1	121	Total O 121 121	0	0
5	2	108	Total O 108 108	0	0
5	3	88	Total O 88 88	0	0
5	4	10	Total O 10 10	0	0

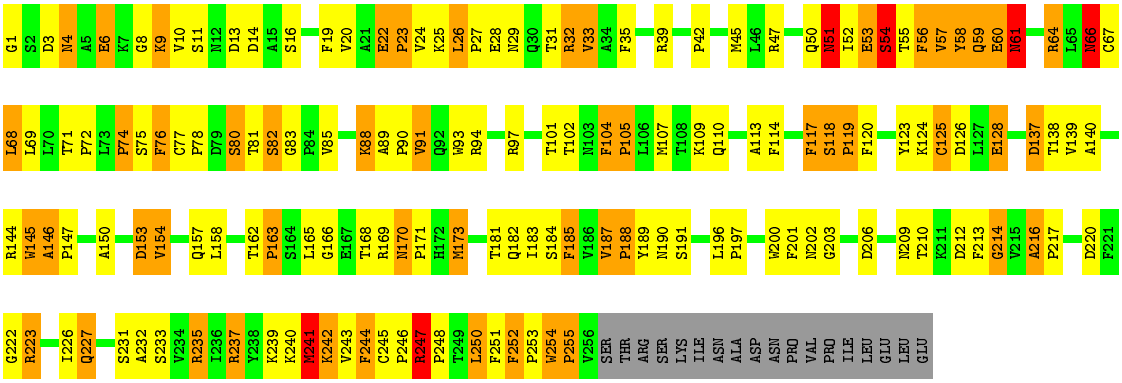
3 Residue-property plots (i)

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.

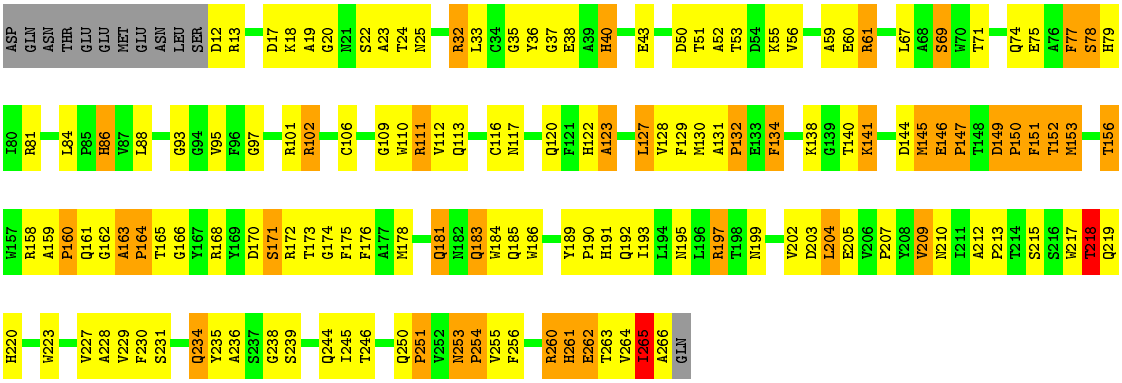
• Molecule 1: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP1)

Chain 1:



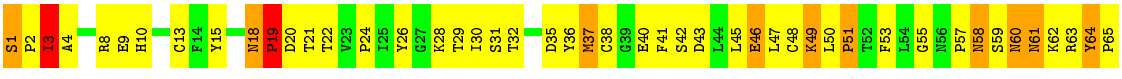
• Molecule 2: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP2)

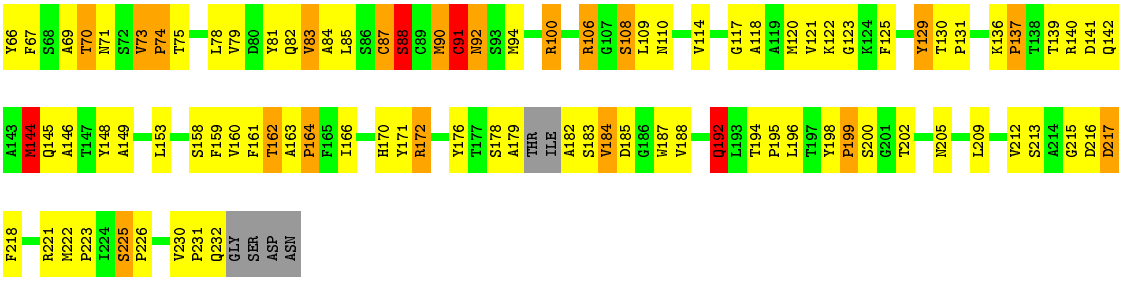
Chain 2:



• Molecule 3: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP3)

Chain 3:





• Molecule 4: THEILER'S MURINE ENCEPHALOMYELITIS VIRUS (SUBUNIT VP4)

Chain 4:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	360.50Å 338.40Å 348.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	46.0 (30.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REAL-SPACE REFINEMENT	Depositor
R, R_{free}	0.300 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6280	wwPDB-VP
Average B, all atoms (Å^2)	0.0	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	2.06	26/2069 (1.3%)	2.32	96/2832 (3.4%)
2	2	2.08	30/2040 (1.5%)	2.31	98/2792 (3.5%)
3	3	2.03	22/1826 (1.2%)	2.29	78/2501 (3.1%)
4	4	2.03	2/194 (1.0%)	2.28	10/262 (3.8%)
All	All	2.06	80/6129 (1.3%)	2.31	282/8387 (3.4%)

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1	GLY	N-CA	9.03	1.59	1.46
3	3	182	ALA	N-CA	8.30	1.62	1.46
1	1	27	PRO	C-N	-7.97	1.15	1.34
3	3	1	SER	N-CA	7.79	1.61	1.46
2	2	146	GLU	C-N	-7.33	1.20	1.34
2	2	254	PRO	C-N	-7.29	1.17	1.34
1	1	254	TRP	C-N	-7.12	1.20	1.34
3	3	131	PRO	C-N	-7.05	1.20	1.34
1	1	90	PRO	C-N	-7.03	1.17	1.34
1	1	216	ALA	C-N	-6.73	1.21	1.34
3	3	153	LEU	C-N	-6.70	1.21	1.33
1	1	184	SER	C-N	-6.58	1.19	1.34
2	2	24	THR	C-N	-6.49	1.19	1.34
3	3	109	LEU	C-N	-6.44	1.19	1.34
1	1	60	GLU	C-N	-6.42	1.19	1.34
1	1	252	PHE	C-N	-6.40	1.22	1.34
1	1	227	GLN	C-N	-6.40	1.21	1.33
2	2	173	THR	C-N	-6.31	1.21	1.33
2	2	160	PRO	C-N	-6.25	1.19	1.34
1	1	126	ASP	C-N	-6.21	1.19	1.34
1	1	187	VAL	C-N	-6.21	1.22	1.34
4	4	35	ASP	C-N	-6.15	1.20	1.34
2	2	162	GLY	N-CA	6.11	1.55	1.46
3	3	79	VAL	C-N	-6.06	1.20	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	251	PHE	C-N	-6.03	1.20	1.34
3	3	215	GLY	C-N	-6.01	1.20	1.34
1	1	226	ILE	C-N	-5.97	1.20	1.34
3	3	69	ALA	C-N	-5.83	1.20	1.34
2	2	147	PRO	C-N	-5.82	1.20	1.34
3	3	81	TYR	C-N	-5.80	1.20	1.34
2	2	78	SER	C-N	-5.80	1.20	1.34
2	2	106	CYS	C-N	-5.75	1.20	1.34
2	2	172	ARG	C-N	-5.75	1.20	1.34
1	1	104	PHE	C-N	-5.65	1.23	1.34
2	2	175	PHE	C-N	-5.65	1.21	1.34
1	1	146	ALA	C-N	-5.58	1.23	1.34
1	1	83	GLY	N-CA	5.47	1.54	1.46
2	2	231	SER	C-N	-5.46	1.23	1.34
2	2	209	VAL	C-N	-5.43	1.21	1.34
2	2	238	GLY	N-CA	5.42	1.54	1.46
2	2	261	HIS	C-N	-5.41	1.21	1.34
1	1	139	VAL	C-N	-5.40	1.21	1.34
1	1	183	ILE	C-N	-5.40	1.21	1.34
3	3	200	SER	C-N	-5.38	1.23	1.33
3	3	137	PRO	C-N	-5.36	1.21	1.34
2	2	190	PRO	C-N	-5.35	1.21	1.34
3	3	38	CYS	C-N	-5.28	1.23	1.33
2	2	246	THR	C-N	-5.28	1.22	1.34
3	3	67	PHE	C-N	-5.27	1.22	1.34
1	1	124	LYS	C-N	-5.26	1.22	1.34
2	2	192	GLN	C-N	-5.22	1.22	1.34
1	1	170	ASN	C-N	-5.20	1.24	1.34
2	2	202	VAL	C-N	-5.20	1.22	1.34
2	2	227	VAL	C-N	-5.19	1.22	1.34
2	2	18	LYS	C-N	-5.18	1.22	1.34
1	1	214	GLY	N-CA	5.18	1.53	1.46
3	3	24	PRO	C-N	-5.16	1.22	1.34
3	3	117	GLY	CA-C	5.16	1.60	1.51
3	3	196	LEU	C-N	-5.13	1.22	1.34
3	3	194	THR	C-N	-5.13	1.24	1.34
1	1	145	TRP	C-N	-5.12	1.22	1.34
1	1	166	GLY	N-CA	5.12	1.53	1.46
3	3	212	VAL	C-N	-5.11	1.22	1.34
2	2	132	PRO	C-N	-5.10	1.22	1.34
2	2	207	PRO	C-N	-5.09	1.22	1.34
4	4	26	TYR	C-N	-5.09	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	3	223	PRO	C-N	-5.08	1.22	1.34
3	3	57	PRO	C-N	-5.08	1.22	1.34
2	2	20	GLY	CA-C	5.07	1.59	1.51
3	3	130	THR	C-N	-5.07	1.24	1.34
1	1	23	PRO	C-N	-5.05	1.22	1.34
1	1	157	GLN	C-N	-5.05	1.22	1.34
2	2	109	GLY	C-N	-5.04	1.22	1.34
2	2	191	HIS	C-N	-5.04	1.22	1.34
1	1	56	PHE	C-N	-5.04	1.22	1.34
2	2	117	ASN	C-N	-5.04	1.22	1.34
3	3	125	PHE	C-N	-5.02	1.22	1.34
2	2	43	GLU	C-N	-5.01	1.22	1.34
2	2	97	GLY	N-CA	5.01	1.53	1.46
2	2	123	ALA	C-N	-5.00	1.24	1.33

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	235	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	1	51	ASN	CB-CA-C	-8.31	93.78	110.40
3	3	106	ARG	NE-CZ-NH2	8.06	124.33	120.30
2	2	260	ARG	NE-CZ-NH2	8.01	124.30	120.30
1	1	223	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	1	97	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	1	237	ARG	NE-CZ-NH2	7.83	124.22	120.30
1	1	64	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	1	39	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	1	144	ARG	NE-CZ-NH2	7.59	124.09	120.30
3	3	221	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	1	247	ARG	NE-CZ-NH2	7.48	124.04	120.30
3	3	172	ARG	NE-CZ-NH2	7.48	124.04	120.30
2	2	13	ARG	NE-CZ-NH2	7.45	124.03	120.30
3	3	8	ARG	NE-CZ-NH2	7.45	124.03	120.30
2	2	111	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	2	61	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	2	81	ARG	NE-CZ-NH2	7.41	124.01	120.30
2	2	32	ARG	NE-CZ-NH2	7.41	124.00	120.30
3	3	140	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	1	169	ARG	NE-CZ-NH2	7.39	124.00	120.30
3	3	100	ARG	NE-CZ-NH2	7.30	123.95	120.30
2	2	101	ARG	NE-CZ-NH2	7.22	123.91	120.30
2	2	197	ARG	NE-CZ-NH2	7.21	123.91	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	47	ARG	NE-CZ-NH2	7.18	123.89	120.30
2	2	158	ARG	NE-CZ-NH2	7.06	123.83	120.30
3	3	63	ARG	NE-CZ-NH2	7.06	123.83	120.30
2	2	102	ARG	NE-CZ-NH2	7.06	123.83	120.30
2	2	168	ARG	NE-CZ-NH2	6.90	123.75	120.30
2	2	172	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	1	94	ARG	NE-CZ-NH2	6.87	123.73	120.30
3	3	218	PHE	N-CA-C	6.86	129.51	111.00
3	3	217	ASP	CB-CA-C	-6.73	96.93	110.40
2	2	43	GLU	O-C-N	6.72	133.46	122.70
1	1	170	ASN	O-C-N	6.69	133.81	121.10
3	3	79	VAL	O-C-N	6.68	133.39	122.70
1	1	32	ARG	NE-CZ-NH2	6.63	123.62	120.30
3	3	53	PHE	N-CA-C	6.54	128.64	111.00
4	4	26	TYR	O-C-N	6.48	133.07	122.70
3	3	226	PRO	O-C-N	6.46	133.03	122.70
2	2	254	PRO	O-C-N	6.40	132.94	122.70
2	2	145	MET	CG-SD-CE	6.39	110.43	100.20
3	3	46	GLU	O-C-N	6.37	132.90	122.70
1	1	173	MET	CG-SD-CE	6.32	110.31	100.20
3	3	94	MET	CG-SD-CE	6.28	110.25	100.20
3	3	90	MET	CG-SD-CE	6.28	110.25	100.20
1	1	113	ALA	O-C-N	6.27	132.73	122.70
3	3	192	GLN	O-C-N	6.24	132.68	122.70
3	3	199	PRO	O-C-N	6.23	132.66	122.70
2	2	235	TYR	O-C-N	6.20	132.62	122.70
3	3	144	MET	CG-SD-CE	6.20	110.12	100.20
1	1	32	ARG	O-C-N	6.20	132.62	122.70
4	4	22	ILE	CB-CA-C	-6.20	99.21	111.60
1	1	242	LYS	O-C-N	6.20	132.61	122.70
1	1	45	MET	CG-SD-CE	6.18	110.09	100.20
3	3	164	PRO	O-C-N	6.18	132.58	122.70
1	1	188	PRO	O-C-N	6.17	132.57	122.70
2	2	189	TYR	O-C-N	6.15	132.78	121.10
1	1	241	MET	CG-SD-CE	6.13	110.02	100.20
3	3	120	MET	CG-SD-CE	6.12	109.99	100.20
2	2	130	MET	CG-SD-CE	6.09	109.94	100.20
2	2	253	ASN	O-C-N	6.09	132.66	121.10
1	1	125	CYS	O-C-N	6.06	132.40	122.70
3	3	37	MET	CG-SD-CE	6.05	109.88	100.20
2	2	153	MET	CG-SD-CE	6.04	109.87	100.20
1	1	137	ASP	O-C-N	6.03	132.35	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	195	PRO	O-C-N	6.01	132.32	122.70
1	1	19	PHE	CB-CA-C	-6.01	98.38	110.40
3	3	149	ALA	O-C-N	6.01	132.31	122.70
3	3	222	MET	CG-SD-CE	6.00	109.80	100.20
1	1	29	ASN	CB-CA-C	-5.99	98.42	110.40
1	1	76	PHE	O-C-N	5.99	132.28	122.70
3	3	142	GLN	O-C-N	5.98	132.27	122.70
2	2	236	ALA	O-C-N	5.98	132.26	122.70
3	3	28	LYS	O-C-N	5.97	132.25	122.70
2	2	78	SER	O-C-N	5.96	132.24	122.70
2	2	111	ARG	O-C-N	5.93	132.19	122.70
1	1	58	TYR	O-C-N	5.93	132.19	122.70
2	2	43	GLU	CB-CA-C	-5.92	98.56	110.40
1	1	107	MET	CG-SD-CE	5.92	109.67	100.20
2	2	174	GLY	O-C-N	5.90	132.15	122.70
2	2	178	MET	CG-SD-CE	5.90	109.63	100.20
3	3	205	ASN	O-C-N	5.88	132.11	122.70
3	3	184	VAL	CB-CA-C	-5.88	100.23	111.40
1	1	26	LEU	O-C-N	5.88	132.27	121.10
2	2	263	THR	O-C-N	5.87	132.10	122.70
1	1	55	THR	O-C-N	5.84	132.04	122.70
2	2	260	ARG	O-C-N	5.81	131.99	122.70
4	4	32	ASN	O-C-N	5.80	131.98	122.70
1	1	47	ARG	O-C-N	5.79	132.09	121.10
1	1	35	PHE	CB-CA-C	-5.78	98.83	110.40
3	3	172	ARG	O-C-N	5.75	131.90	122.70
1	1	10	VAL	O-C-N	5.74	131.89	122.70
1	1	140	ALA	O-C-N	5.74	131.88	122.70
2	2	106	CYS	O-C-N	5.73	131.87	122.70
2	2	172	ARG	O-C-N	5.73	131.87	122.70
1	1	126	ASP	O-C-N	5.73	131.86	122.70
4	4	35	ASP	O-C-N	5.72	131.85	122.70
1	1	91	VAL	O-C-N	5.71	131.83	122.70
2	2	159	ALA	O-C-N	5.70	131.93	121.10
3	3	50	LEU	O-C-N	5.70	131.93	121.10
1	1	157	GLN	CB-CA-C	-5.67	99.06	110.40
2	2	95	VAL	O-C-N	5.66	131.76	122.70
1	1	206	ASP	O-C-N	5.66	131.76	122.70
4	4	28	ASN	CB-CA-C	-5.65	99.10	110.40
2	2	120	GLN	O-C-N	5.65	131.74	122.70
3	3	129	TYR	O-C-N	5.64	131.73	122.70
3	3	163	ALA	O-C-N	5.64	131.82	121.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	3	69	ALA	O-C-N	5.64	131.72	122.70
3	3	64	TYR	O-C-N	5.63	131.81	121.10
3	3	74	PRO	O-C-N	5.62	131.70	122.70
1	1	61	ASN	O-C-N	5.62	131.69	122.70
3	3	160	VAL	O-C-N	5.62	131.69	122.70
2	2	192	GLN	O-C-N	5.61	131.68	122.70
2	2	163	ALA	O-C-N	5.61	131.75	121.10
2	2	228	ALA	O-C-N	5.61	131.67	122.70
2	2	158	ARG	O-C-N	5.61	131.67	122.70
2	2	75	GLU	O-C-N	5.60	131.65	122.70
1	1	22	GLU	O-C-N	5.59	131.73	121.10
2	2	113	GLN	O-C-N	5.59	131.65	122.70
1	1	51	ASN	O-C-N	5.59	131.64	122.70
2	2	129	PHE	N-CA-C	5.59	126.09	111.00
3	3	2	PRO	O-C-N	5.58	131.62	122.70
1	1	89	ALA	O-C-N	5.58	131.69	121.10
4	4	33	SER	O-C-N	5.58	131.62	122.70
2	2	146	GLU	O-C-N	5.57	131.69	121.10
2	2	50	ASP	O-C-N	5.57	131.61	122.70
3	3	125	PHE	CB-CA-C	-5.57	99.26	110.40
3	3	213	SER	O-C-N	5.55	131.58	122.70
2	2	190	PRO	O-C-N	5.51	131.51	122.70
1	1	71	THR	O-C-N	5.50	131.56	121.10
4	4	38	ALA	O-C-N	5.50	131.50	122.70
2	2	244	GLN	O-C-N	5.49	131.49	122.70
1	1	19	PHE	N-CA-C	5.47	125.78	111.00
1	1	27	PRO	O-C-N	5.47	131.45	122.70
2	2	160	PRO	O-C-N	5.47	131.44	122.70
2	2	205	GLU	O-C-N	5.46	131.44	122.70
3	3	171	TYR	O-C-N	5.46	131.43	122.70
2	2	151	PHE	N-CA-C	5.46	125.73	111.00
1	1	59	GLN	O-C-N	5.45	131.43	122.70
2	2	156	THR	O-C-N	5.45	131.43	122.70
3	3	3	ILE	O-C-N	5.45	131.42	122.70
3	3	58	ASN	CB-CA-C	-5.45	99.50	110.40
2	2	55	LYS	O-C-N	5.45	131.42	122.70
1	1	244	PHE	CB-CA-C	-5.45	99.50	110.40
1	1	53	GLU	O-C-N	5.45	131.41	122.70
2	2	134	PHE	CB-CA-C	-5.45	99.51	110.40
2	2	149	ASP	O-C-N	5.45	131.44	121.10
1	1	231	SER	O-C-N	5.44	131.41	122.70
1	1	19	PHE	O-C-N	5.43	131.40	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	262	GLU	N-CA-C	5.43	125.67	111.00
3	3	109	LEU	O-C-N	5.42	131.38	122.70
1	1	170	ASN	CB-CA-C	-5.42	99.55	110.40
2	2	13	ARG	CA-C-N	-5.42	105.27	117.20
2	2	131	ALA	O-C-N	5.42	131.40	121.10
3	3	146	ALA	O-C-N	5.42	131.37	122.70
1	1	222	GLY	O-C-N	5.42	131.37	122.70
2	2	77	PHE	N-CA-C	5.41	125.61	111.00
1	1	157	GLN	O-C-N	5.41	131.35	122.70
3	3	202	THR	O-C-N	5.41	131.37	121.10
2	2	69	SER	O-C-N	5.40	131.35	122.70
1	1	153	ASP	O-C-N	5.40	131.34	122.70
2	2	202	VAL	O-C-N	5.40	131.34	122.70
1	1	90	PRO	O-C-N	5.40	131.34	122.70
1	1	147	PRO	O-C-N	5.39	131.33	122.70
2	2	17	ASP	O-C-N	5.38	131.30	122.70
2	2	122	HIS	O-C-N	5.38	131.30	122.70
2	2	74	GLN	O-C-N	5.37	131.30	122.70
1	1	54	SER	O-C-N	5.37	131.29	122.70
3	3	29	THR	O-C-N	5.37	131.29	122.70
2	2	244	GLN	CB-CA-C	-5.36	99.69	110.40
1	1	72	PRO	CA-C-N	-5.35	105.43	117.20
1	1	88	LYS	O-C-N	5.35	131.25	122.70
1	1	6	GLU	O-C-N	5.34	131.25	122.70
1	1	232	ALA	O-C-N	5.34	131.25	122.70
3	3	51	PRO	O-C-N	5.34	131.24	122.70
2	2	128	VAL	O-C-N	5.33	131.23	122.70
2	2	227	VAL	O-C-N	5.33	131.22	122.70
1	1	78	PRO	O-C-N	5.32	131.22	122.70
3	3	140	ARG	O-C-N	5.32	131.21	122.70
3	3	60	ASN	CA-C-N	-5.32	105.51	117.20
3	3	114	VAL	O-C-N	5.31	131.20	122.70
1	1	67	CYS	O-C-N	5.31	131.20	122.70
1	1	182	GLN	O-C-N	5.30	131.19	122.70
1	1	210	THR	O-C-N	5.30	131.18	122.70
2	2	147	PRO	O-C-N	5.29	131.17	122.70
3	3	92	ASN	N-CA-C	5.29	125.29	111.00
2	2	246	THR	O-C-N	5.29	131.16	122.70
3	3	81	TYR	O-C-N	5.29	131.16	122.70
3	3	162	THR	O-C-N	5.29	131.16	122.70
3	3	88	SER	N-CA-C	5.29	125.27	111.00
1	1	197	PRO	O-C-N	5.28	131.15	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	150	PRO	O-C-N	5.27	131.14	122.70
3	3	63	ARG	N-CA-C	5.27	125.23	111.00
1	1	220	ASP	O-C-N	5.27	131.13	122.70
3	3	225	SER	O-C-N	5.27	131.11	121.10
2	2	255	VAL	O-C-N	5.26	131.12	122.70
2	2	22	SER	O-C-N	5.26	131.11	122.70
3	3	19	PRO	O-C-N	5.25	131.10	122.70
2	2	261	HIS	O-C-N	5.25	131.10	122.70
2	2	265	ILE	CB-CA-C	-5.25	101.10	111.60
3	3	1	SER	O-C-N	5.25	131.08	121.10
3	3	188	VAL	O-C-N	5.24	131.08	122.70
3	3	131	PRO	O-C-N	5.23	131.04	121.10
2	2	32	ARG	O-C-N	5.22	131.06	122.70
2	2	140	THR	O-C-N	5.22	131.06	122.70
1	1	250	LEU	O-C-N	5.22	131.05	122.70
1	1	123	TYR	O-C-N	5.21	131.04	122.70
2	2	116	CYS	O-C-N	5.21	131.04	122.70
3	3	166	ILE	O-C-N	5.20	131.01	122.70
2	2	132	PRO	O-C-N	5.19	131.01	122.70
1	1	150	ALA	O-C-N	5.18	130.95	121.10
3	3	73	VAL	O-C-N	5.18	130.95	121.10
1	1	196	LEU	O-C-N	5.18	130.94	121.10
1	1	57	VAL	O-C-N	5.18	130.99	122.70
1	1	185	PHE	O-C-N	5.18	130.99	122.70
1	1	163	PRO	O-C-N	5.18	130.98	122.70
2	2	52	ALA	O-C-N	5.18	130.98	122.70
2	2	250	GLN	O-C-N	5.17	130.92	121.10
1	1	74	PRO	O-C-N	5.16	130.96	122.70
1	1	128	GLU	O-C-N	5.16	130.96	122.70
1	1	66	ASN	CA-C-N	-5.16	105.85	117.20
2	2	23	ALA	O-C-N	5.16	130.95	122.70
2	2	127	LEU	O-C-N	5.16	130.95	122.70
2	2	150	PRO	CA-C-N	-5.16	105.86	117.20
1	1	9	LYS	O-C-N	5.15	130.95	122.70
2	2	262	GLU	O-C-N	5.15	130.94	122.70
1	1	22	GLU	N-CA-C	5.15	124.90	111.00
1	1	105	PRO	O-C-N	5.15	130.94	122.70
3	3	13	CYS	O-C-N	5.15	130.94	122.70
3	3	148	TYR	O-C-N	5.15	130.94	122.70
2	2	256	PHE	N-CA-C	5.15	124.90	111.00
1	1	209	ASN	CB-CA-C	-5.15	100.10	110.40
2	2	40	HIS	O-C-N	5.14	130.93	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	215	SER	N-CA-C	5.13	124.85	111.00
2	2	239	SER	O-C-N	5.13	130.91	122.70
3	3	139	THR	O-C-N	5.12	130.89	122.70
3	3	230	VAL	O-C-N	5.12	130.83	121.10
1	1	191	SER	O-C-N	5.11	130.81	121.10
3	3	110	ASN	O-C-N	5.11	130.88	122.70
2	2	176	PHE	N-CA-C	5.11	124.79	111.00
3	3	194	THR	O-C-N	5.11	130.81	121.10
2	2	220	HIS	O-C-N	5.10	130.86	122.70
3	3	161	PHE	O-C-N	5.10	130.86	122.70
1	1	76	PHE	CB-CA-C	-5.09	100.22	110.40
2	2	229	VAL	O-C-N	5.09	130.85	122.70
2	2	203	ASP	O-C-N	5.09	130.84	122.70
3	3	141	ASP	O-C-N	5.07	130.81	122.70
2	2	204	LEU	O-C-N	5.07	130.81	122.70
3	3	137	PRO	O-C-N	5.07	130.81	122.70
2	2	170	ASP	O-C-N	5.06	130.80	122.70
1	1	209	ASN	O-C-N	5.06	130.80	122.70
3	3	118	ALA	O-C-N	5.06	130.80	122.70
1	1	72	PRO	O-C-N	5.06	130.79	122.70
2	2	234	GLN	O-C-N	5.06	130.79	122.70
3	3	4	ALA	O-C-N	5.05	130.78	122.70
2	2	112	VAL	CB-CA-C	-5.05	101.80	111.40
1	1	233	SER	O-C-N	5.05	130.78	122.70
4	4	25	PHE	CB-CA-C	-5.05	100.30	110.40
4	4	30	TYR	O-C-N	5.05	130.78	122.70
2	2	51	THR	O-C-N	5.05	130.78	122.70
4	4	23	ASN	N-CA-C	5.05	124.63	111.00
2	2	24	THR	O-C-N	5.04	130.77	122.70
2	2	251	PRO	O-C-N	5.04	130.77	122.70
1	1	124	LYS	O-C-N	5.04	130.76	122.70
3	3	70	THR	O-C-N	5.04	130.76	122.70
1	1	181	THR	N-CA-C	5.04	124.60	111.00
1	1	244	PHE	N-CA-C	5.03	124.59	111.00
3	3	49	LYS	O-C-N	5.03	130.75	122.70
1	1	139	VAL	CB-CA-C	-5.03	101.84	111.40
3	3	159	PHE	O-C-N	5.03	130.74	122.70
1	1	4	ASN	CB-CA-C	-5.02	100.35	110.40
3	3	110	ASN	CB-CA-C	-5.02	100.35	110.40
2	2	59	ALA	O-C-N	5.02	130.73	122.70
3	3	123	GLY	O-C-N	5.02	130.73	122.70
1	1	39	ARG	O-C-N	5.01	130.71	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	168	THR	O-C-N	5.01	130.72	122.70
2	2	71	THR	O-C-N	5.01	130.71	122.70
1	1	117	PHE	N-CA-C	5.01	124.52	111.00
2	2	53	THR	O-C-N	5.01	130.71	122.70
1	1	31	THR	O-C-N	5.00	130.71	122.70
1	1	35	PHE	O-C-N	5.00	130.70	122.70

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	1	2005	0	1947	104	0
2	2	1982	0	1869	104	0
3	3	1774	0	1729	100	0
4	4	192	0	171	17	0
5	1	121	0	0	8	0
5	2	108	0	0	13	0
5	3	88	0	0	4	0
5	4	10	0	0	0	0
All	All	6280	0	5716	298	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 26.

All (298) 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)
2:2:127:LEU:HB2	2:2:230:PHE:CZ	1.60	1.34
2:2:127:LEU:HB2	2:2:230:PHE:CE2	1.75	1.21
2:2:163:ALA:CB	3:3:232:GLN:HG3	1.73	1.16
2:2:141:LYS:HD3	2:2:144:ASP:OD2	1.45	1.16
2:2:163:ALA:HB2	3:3:232:GLN:HG3	1.16	1.14
1:1:22:GLU:HB2	1:1:23:PRO:HD2	1.33	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:141:LYS:HG2	2:2:141:LYS:O	1.59	1.01
2:2:183:GLN:HE21	2:2:183:GLN:H	1.06	1.00
2:2:127:LEU:CB	2:2:230:PHE:CZ	2.44	0.99
1:1:223:ARG:NH1	5:1:336:HOH:O	1.96	0.98
1:1:14:ASP:HB2	3:3:217:ASP:OD2	1.64	0.98
3:3:172:ARG:HD3	5:3:295:HOH:O	1.64	0.96
2:2:219:GLN:HB3	5:2:328:HOH:O	1.64	0.96
2:2:218:THR:HG23	5:2:328:HOH:O	1.66	0.94
1:1:154:VAL:HG12	1:1:154:VAL:O	1.65	0.94
3:3:58:ASN:O	3:3:61:ASN:HA	1.70	0.91
1:1:22:GLU:HB2	1:1:23:PRO:CD	2.00	0.91
2:2:127:LEU:HD22	2:2:230:PHE:HZ	1.38	0.89
3:3:144:MET:HE2	3:3:145:GLN:NE2	1.88	0.89
2:2:161:GLN:HE21	2:2:164:PRO:HA	1.34	0.89
2:2:138:LYS:NZ	2:2:152:THR:HG22	1.88	0.89
2:2:218:THR:HB	5:2:354:HOH:O	1.72	0.88
3:3:61:ASN:O	3:3:61:ASN:ND2	2.07	0.87
1:1:50:GLN:NE2	1:1:57:VAL:H	1.72	0.87
2:2:161:GLN:HE22	2:2:166:GLY:H	1.23	0.87
2:2:264:VAL:O	2:2:264:VAL:HG12	1.75	0.86
1:1:68:LEU:C	1:1:68:LEU:HD12	1.95	0.85
2:2:127:LEU:CB	2:2:230:PHE:CE2	2.58	0.84
2:2:141:LYS:CD	2:2:144:ASP:OD2	2.24	0.83
3:3:58:ASN:O	3:3:61:ASN:N	2.11	0.83
4:4:22:ILE:O	4:4:22:ILE:HG22	1.79	0.83
3:3:179:ALA:O	3:3:183:SER:HA	1.79	0.83
1:1:154:VAL:CG1	1:1:154:VAL:O	2.26	0.82
3:3:144:MET:O	3:3:144:MET:HG2	1.77	0.82
2:2:141:LYS:HD2	2:2:144:ASP:HB2	1.60	0.82
1:1:22:GLU:CB	1:1:23:PRO:HD2	2.08	0.82
1:1:59:GLN:H	1:1:66:ASN:HD21	1.30	0.80
3:3:74:PRO:HD2	3:3:192:GLN:HG3	1.61	0.80
4:4:20:VAL:O	4:4:23:ASN:HB3	1.83	0.79
1:1:11:SER:OG	1:1:13:ASP:OD1	2.00	0.78
3:3:59:SER:C	3:3:61:ASN:H	1.85	0.77
2:2:138:LYS:HZ3	2:2:152:THR:HG22	1.47	0.76
1:1:145:TRP:HE3	1:1:171:PRO:HG2	1.49	0.75
3:3:144:MET:CE	3:3:145:GLN:NE2	2.49	0.74
2:2:212:ALA:HB1	2:2:213:PRO:HD2	1.70	0.74
2:2:218:THR:CG2	5:2:328:HOH:O	2.30	0.74
1:1:59:GLN:H	1:1:66:ASN:ND2	1.85	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:163:ALA:CB	3:3:232:GLN:CG	2.61	0.73
3:3:58:ASN:O	3:3:61:ASN:CA	2.35	0.73
3:3:78:LEU:HD11	3:3:192:GLN:HG2	1.69	0.73
2:2:127:LEU:HD22	2:2:230:PHE:CZ	2.21	0.73
2:2:183:GLN:HE21	2:2:183:GLN:N	1.85	0.73
2:2:156:THR:HB	5:2:370:HOH:O	1.89	0.73
2:2:264:VAL:HA	5:2:345:HOH:O	1.88	0.73
4:4:24:ASN:O	4:4:26:TYR:N	2.22	0.73
3:3:179:ALA:O	3:3:183:SER:CA	2.36	0.72
1:1:145:TRP:CE3	1:1:171:PRO:HG2	2.24	0.72
3:3:176:TYR:CE1	3:3:179:ALA:O	2.43	0.72
3:3:185:ASP:OD2	5:3:304:HOH:O	2.08	0.71
3:3:176:TYR:HE1	3:3:179:ALA:O	1.72	0.71
3:3:84:ALA:HA	5:3:304:HOH:O	1.91	0.70
1:1:247:ARG:HB2	1:1:248:PRO:HD2	1.73	0.70
2:2:265:ILE:HG22	2:2:266:ALA:N	2.06	0.69
4:4:24:ASN:ND2	4:4:24:ASN:H	1.90	0.69
1:1:52:ILE:HG12	1:1:163:PRO:HG3	1.74	0.69
1:1:16:SER:HB3	1:1:22:GLU:HA	1.75	0.69
4:4:24:ASN:HD22	4:4:25:PHE:H	1.38	0.69
1:1:51:ASN:HB3	1:1:53:GLU:H	1.55	0.69
1:1:22:GLU:CB	1:1:23:PRO:CD	2.64	0.68
3:3:61:ASN:CG	3:3:61:ASN:O	2.29	0.68
2:2:163:ALA:HB1	3:3:232:GLN:HG3	1.72	0.67
2:2:183:GLN:NE2	2:2:183:GLN:H	1.85	0.67
3:3:84:ALA:O	3:3:87:CYS:N	2.27	0.67
2:2:127:LEU:HD13	2:2:230:PHE:CE2	2.29	0.67
2:2:127:LEU:CD2	2:2:230:PHE:HZ	2.08	0.67
1:1:61:ASN:ND2	1:1:64:ARG:HH21	1.92	0.67
4:4:21:ILE:C	4:4:23:ASN:H	1.98	0.67
1:1:14:ASP:C	1:1:14:ASP:OD1	2.33	0.67
1:1:165:LEU:HD12	1:1:227:GLN:HB2	1.77	0.67
2:2:77:PHE:CE2	3:3:65:PRO:HG3	2.30	0.66
3:3:61:ASN:HD22	3:3:61:ASN:C	1.98	0.66
3:3:59:SER:C	3:3:61:ASN:N	2.47	0.66
2:2:127:LEU:HD13	2:2:230:PHE:CZ	2.31	0.66
2:2:161:GLN:NE2	2:2:164:PRO:HA	2.08	0.65
3:3:136:LYS:HB2	3:3:187:TRP:CE2	2.30	0.65
2:2:77:PHE:O	2:2:79:HIS:HD2	1.79	0.65
1:1:61:ASN:C	1:1:61:ASN:HD22	2.00	0.65
3:3:61:ASN:C	3:3:61:ASN:ND2	2.49	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:84:ALA:O	3:3:87:CYS:HB3	1.98	0.64
1:1:68:LEU:CD1	1:1:68:LEU:C	2.66	0.64
3:3:18:ASN:HD22	3:3:19:PRO:CD	2.12	0.63
1:1:24:VAL:N	3:3:217:ASP:OD1	2.31	0.63
2:2:163:ALA:HB2	3:3:232:GLN:CG	2.11	0.63
3:3:82:GLN:NE2	3:3:184:VAL:HG11	2.14	0.62
3:3:18:ASN:HD22	3:3:19:PRO:N	1.96	0.62
3:3:45:LEU:O	3:3:48:CYS:HB2	1.98	0.62
2:2:146:GLU:HB3	2:2:147:PRO:HD2	1.80	0.62
2:2:127:LEU:CG	2:2:230:PHE:CZ	2.82	0.62
3:3:18:ASN:HD22	3:3:19:PRO:HD2	1.65	0.62
3:3:162:THR:O	3:3:164:PRO:HD3	1.99	0.62
3:3:144:MET:HE2	3:3:145:GLN:CD	2.20	0.61
3:3:179:ALA:O	3:3:183:SER:N	2.32	0.61
3:3:43:ASP:O	3:3:46:GLU:HG3	1.99	0.61
3:3:176:TYR:HE1	3:3:183:SER:HA	1.64	0.61
3:3:88:SER:O	3:3:91:CYS:HB2	2.01	0.61
1:1:51:ASN:HB2	1:1:54:SER:OG	2.02	0.60
3:3:136:LYS:HG3	3:3:137:PRO:HD2	1.84	0.60
3:3:18:ASN:ND2	3:3:19:PRO:HD2	2.17	0.59
1:1:119:PRO:HB2	3:3:47:LEU:HD13	1.85	0.58
3:3:144:MET:CE	3:3:145:GLN:CD	2.72	0.58
1:1:118:SER:C	1:1:120:PHE:H	2.06	0.58
1:1:145:TRP:CG	1:1:146:ALA:N	2.72	0.58
2:2:181:GLN:CG	2:2:186:TRP:HE1	2.18	0.57
1:1:162:THR:HB	1:1:163:PRO:HD2	1.87	0.56
2:2:102:ARG:NH2	5:2:352:HOH:O	2.24	0.56
1:1:54:SER:O	1:1:227:GLN:NE2	2.38	0.56
1:1:3:ASP:OD1	1:1:4:ASN:N	2.27	0.56
1:1:6:GLU:HA	2:2:193:ILE:HB	1.88	0.56
2:2:264:VAL:CA	5:2:345:HOH:O	2.51	0.56
1:1:255:PRO:HG3	3:3:88:SER:HB2	1.87	0.56
2:2:165:THR:HG22	3:3:231:PRO:HB2	1.88	0.55
2:2:163:ALA:HB1	3:3:232:GLN:CG	2.32	0.55
3:3:108:SER:OG	3:3:217:ASP:OD2	2.25	0.55
4:4:24:ASN:O	4:4:26:TYR:O	2.25	0.55
1:1:119:PRO:CB	3:3:47:LEU:HD13	2.36	0.55
3:3:172:ARG:CZ	3:3:185:ASP:HB3	2.37	0.55
1:1:128:GLU:HB3	1:1:237:ARG:HB3	1.88	0.55
1:1:101:THR:HG22	1:1:102:THR:N	2.21	0.55
2:2:67:LEU:HB2	2:2:245:ILE:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:23:PRO:HA	3:3:217:ASP:OD1	2.06	0.54
2:2:127:LEU:CD2	2:2:230:PHE:CZ	2.88	0.54
3:3:84:ALA:O	3:3:87:CYS:CB	2.55	0.54
1:1:117:PHE:CE1	1:1:119:PRO:HG3	2.43	0.54
1:1:56:PHE:C	1:1:56:PHE:CD1	2.81	0.54
1:1:247:ARG:NH2	5:1:308:HOH:O	2.40	0.54
3:3:88:SER:HA	5:3:316:HOH:O	2.08	0.54
2:2:138:LYS:NZ	2:2:149:ASP:O	2.41	0.54
3:3:83:VAL:HG21	3:3:129:TYR:CE1	2.43	0.54
3:3:74:PRO:HG2	3:3:78:LEU:HD21	1.90	0.53
2:2:264:VAL:O	2:2:264:VAL:CG1	2.47	0.53
1:1:250:LEU:HD21	3:3:231:PRO:HG3	1.91	0.53
2:2:217:TRP:CG	2:2:218:THR:N	2.77	0.52
2:2:261:HIS:HD2	5:2:279:HOH:O	1.92	0.52
3:3:90:MET:O	3:3:92:ASN:N	2.43	0.52
3:3:3:ILE:CD1	3:3:3:ILE:N	2.73	0.52
3:3:106:ARG:HH12	3:3:170:HIS:HD2	1.57	0.52
3:3:70:THR:OG1	3:3:71:ASN:N	2.41	0.52
3:3:20:ASP:OD1	3:3:21:THR:N	2.40	0.52
1:1:201:PHE:O	1:1:203:GLY:N	2.39	0.52
1:1:42:PRO:HA	1:1:235:ARG:HB3	1.91	0.52
2:2:141:LYS:CD	2:2:144:ASP:HB2	2.37	0.51
3:3:62:LYS:HD3	3:3:64:TYR:OH	2.10	0.51
3:3:59:SER:O	3:3:61:ASN:N	2.44	0.51
3:3:64:TYR:C	3:3:66:TYR:H	2.12	0.51
3:3:176:TYR:CZ	3:3:179:ALA:HA	2.46	0.51
3:3:66:TYR:HB3	3:3:209:LEU:HA	1.91	0.51
1:1:61:ASN:C	1:1:61:ASN:ND2	2.64	0.51
2:2:218:THR:CG2	2:2:219:GLN:N	2.73	0.51
1:1:42:PRO:HG3	1:1:235:ARG:NH1	2.26	0.50
1:1:223:ARG:NE	5:1:351:HOH:O	2.19	0.50
1:1:244:PHE:CD1	1:1:244:PHE:N	2.80	0.50
3:3:9:GLU:HG2	3:3:10:HIS:N	2.26	0.50
1:1:244:PHE:CD2	3:3:40:GLU:HB2	2.45	0.50
1:1:240:LYS:HG3	1:1:240:LYS:O	2.11	0.50
1:1:119:PRO:HB2	3:3:47:LEU:CD1	2.41	0.50
2:2:127:LEU:CD1	2:2:230:PHE:CE2	2.94	0.50
4:4:21:ILE:O	4:4:23:ASN:N	2.42	0.50
1:1:76:PHE:CG	1:1:77:CYS:N	2.79	0.50
2:2:40:HIS:O	2:2:253:ASN:ND2	2.37	0.50
2:2:33:LEU:HB3	2:2:204:LEU:HD23	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:247:ARG:HB2	1:1:248:PRO:CD	2.39	0.49
3:3:136:LYS:HD2	3:3:187:TRP:CD1	2.47	0.49
2:2:127:LEU:CD1	2:2:230:PHE:CZ	2.96	0.49
2:2:25:ASN:ND2	5:2:348:HOH:O	2.38	0.49
1:1:118:SER:O	1:1:120:PHE:N	2.44	0.49
3:3:49:LYS:O	3:3:51:PRO:HD3	2.12	0.49
4:4:29:GLN:HG3	4:4:34:ILE:HD11	1.94	0.49
3:3:31:SER:HB2	4:4:33:SER:HB2	1.95	0.49
2:2:251:PRO:HB2	2:2:254:PRO:HG3	1.95	0.49
3:3:106:ARG:HH12	3:3:170:HIS:CD2	2.31	0.48
2:2:138:LYS:CE	2:2:152:THR:HG22	2.42	0.48
1:1:76:PHE:O	1:1:77:CYS:C	2.52	0.48
1:1:109:LYS:O	1:1:110:GLN:HB3	2.13	0.48
3:3:18:ASN:C	3:3:18:ASN:HD22	2.17	0.48
2:2:260:ARG:HH11	2:2:260:ARG:HG3	1.78	0.48
1:1:68:LEU:HB2	5:1:362:HOH:O	2.14	0.48
2:2:181:GLN:HG3	2:2:186:TRP:HE1	1.78	0.48
1:1:200:TRP:CH2	1:1:214:GLY:HA3	2.49	0.48
3:3:198:TYR:HB2	3:3:199:PRO:HD2	1.95	0.48
4:4:31:GLN:O	4:4:31:GLN:HG3	2.13	0.48
2:2:181:GLN:HG2	2:2:186:TRP:HE1	1.79	0.47
1:1:125:CYS:HB3	1:1:241:MET:HA	1.96	0.47
2:2:132:PRO:HD3	2:2:223:TRP:CZ3	2.49	0.47
1:1:68:LEU:O	1:1:68:LEU:HD12	2.12	0.47
1:1:68:LEU:O	1:1:223:ARG:HB2	2.15	0.47
3:3:82:GLN:O	3:3:84:ALA:N	2.48	0.47
1:1:60:GLU:HG2	1:1:61:ASN:N	2.28	0.47
1:1:114:PHE:C	1:1:114:PHE:CD1	2.88	0.47
2:2:127:LEU:CG	2:2:230:PHE:HZ	2.26	0.47
2:2:163:ALA:O	2:2:165:THR:N	2.46	0.47
3:3:43:ASP:OD1	3:3:45:LEU:HB2	2.15	0.47
4:4:22:ILE:O	4:4:24:ASN:ND2	2.48	0.47
2:2:32:ARG:HH21	2:2:111:ARG:HD3	1.79	0.47
1:1:32:ARG:O	1:1:33:VAL:C	2.53	0.47
2:2:102:ARG:HG2	2:2:262:GLU:HB2	1.96	0.47
1:1:74:PRO:HA	1:1:110:GLN:HB3	1.97	0.46
1:1:80:SER:C	1:1:82:SER:N	2.68	0.46
2:2:123:ALA:HB3	2:2:234:GLN:HB2	1.97	0.46
1:1:66:ASN:ND2	5:1:378:HOH:O	2.48	0.46
4:4:23:ASN:O	4:4:23:ASN:CG	2.51	0.46
2:2:56:VAL:O	2:2:60:GLU:HG3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:144:ASP:O	2:2:145:MET:HB2	2.14	0.46
2:2:146:GLU:HB3	2:2:147:PRO:CD	2.46	0.46
1:1:255:PRO:CG	3:3:88:SER:HB2	2.46	0.46
2:2:88:LEU:O	2:2:93:GLY:HA3	2.16	0.46
3:3:40:GLU:CG	3:3:41:PHE:N	2.79	0.46
2:2:33:LEU:C	2:2:33:LEU:HD13	2.37	0.46
1:1:85:VAL:HG12	1:1:88:LYS:HG3	1.97	0.46
2:2:199:ASN:OD1	2:2:199:ASN:N	2.49	0.45
2:2:161:GLN:HE22	2:2:166:GLY:N	2.03	0.45
1:1:8:GLY:O	1:1:9:LYS:HB3	2.16	0.45
2:2:84:LEU:HB3	2:2:110:TRP:CZ2	2.51	0.45
1:1:33:VAL:HG11	1:1:243:VAL:HG22	1.99	0.45
4:4:17:ASN:O	4:4:17:ASN:CG	2.55	0.45
2:2:149:ASP:N	2:2:150:PRO:CD	2.80	0.45
1:1:223:ARG:NH2	5:1:351:HOH:O	2.50	0.45
2:2:264:VAL:C	5:2:345:HOH:O	2.55	0.45
1:1:60:GLU:CG	1:1:61:ASN:N	2.80	0.45
1:1:25:LYS:HG3	1:1:26:LEU:N	2.32	0.44
3:3:90:MET:O	3:3:91:CYS:C	2.56	0.44
1:1:66:ASN:N	1:1:66:ASN:HD22	2.16	0.44
3:3:176:TYR:CE1	3:3:183:SER:HA	2.48	0.44
2:2:171:SER:HA	5:2:367:HOH:O	2.18	0.44
3:3:18:ASN:C	3:3:20:ASP:H	2.19	0.44
1:1:188:PRO:O	1:1:190:ASN:N	2.50	0.44
3:3:176:TYR:HE1	3:3:183:SER:CA	2.31	0.44
1:1:14:ASP:HB3	3:3:216:ASP:HB3	1.99	0.44
3:3:91:CYS:O	3:3:100:ARG:NH2	2.50	0.44
1:1:3:ASP:CG	1:1:4:ASN:H	2.12	0.44
1:1:153:ASP:CG	1:1:153:ASP:O	2.56	0.44
2:2:127:LEU:HD13	2:2:230:PHE:HE2	1.79	0.43
3:3:15:TYR:HB2	3:3:18:ASN:HB2	1.99	0.43
1:1:137:ASP:O	1:1:138:THR:C	2.55	0.43
1:1:254:TRP:CH2	3:3:55:GLY:HA3	2.53	0.43
2:2:209:VAL:O	2:2:210:ASN:HB2	2.17	0.43
2:2:144:ASP:O	2:2:145:MET:CB	2.66	0.43
1:1:51:ASN:O	1:1:227:GLN:HG2	2.19	0.43
1:1:117:PHE:CZ	1:1:119:PRO:HG3	2.53	0.43
2:2:19:ALA:HB1	2:2:61:ARG:HA	2.00	0.43
2:2:35:GLY:C	2:2:37:GLY:N	2.72	0.43
2:2:86:HIS:H	2:2:86:HIS:CD2	2.36	0.43
2:2:164:PRO:HG3	2:2:183:GLN:NE2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:76:PHE:HB3	1:1:93:TRP:CE2	2.53	0.43
2:2:78:SER:HA	2:2:160:PRO:HD3	2.01	0.43
2:2:217:TRP:CD2	2:2:218:THR:N	2.87	0.43
1:1:252:PHE:CG	1:1:253:PRO:HD2	2.54	0.43
1:1:213:PHE:CZ	2:2:150:PRO:HB3	2.54	0.43
1:1:185:PHE:HA	3:3:22:THR:HG23	2.01	0.42
1:1:66:ASN:H	1:1:66:ASN:HD22	1.66	0.42
2:2:32:ARG:NH2	2:2:111:ARG:HD3	2.35	0.42
4:4:23:ASN:HD22	4:4:23:ASN:N	2.17	0.42
1:1:223:ARG:CZ	5:1:351:HOH:O	2.64	0.42
1:1:170:ASN:HB3	1:1:171:PRO:HD2	2.01	0.42
1:1:252:PHE:HA	1:1:253:PRO:HD3	1.91	0.42
1:1:245:CYS:HB3	2:2:36:TYR:OH	2.19	0.42
2:2:149:ASP:N	2:2:150:PRO:HD3	2.35	0.42
1:1:254:TRP:HZ2	2:2:184:TRP:CE2	2.38	0.42
3:3:198:TYR:HB2	3:3:199:PRO:CD	2.50	0.42
1:1:80:SER:O	1:1:82:SER:N	2.53	0.42
1:1:125:CYS:HB2	1:1:239:LYS:O	2.20	0.42
3:3:82:GLN:CD	3:3:184:VAL:HG11	2.40	0.42
4:4:25:PHE:HB3	4:4:26:TYR:H	1.74	0.42
2:2:138:LYS:HE2	2:2:152:THR:CG2	2.50	0.41
1:1:248:PRO:HB3	2:2:185:GLN:HB2	2.01	0.41
1:1:216:ALA:HA	1:1:217:PRO:HD3	1.88	0.41
2:2:127:LEU:HD13	2:2:230:PHE:HZ	1.83	0.41
1:1:68:LEU:HD12	1:1:69:LEU:N	2.32	0.41
2:2:265:ILE:O	2:2:266:ALA:C	2.59	0.41
3:3:121:VAL:HG12	3:3:122:LYS:N	2.34	0.41
2:2:265:ILE:N	5:2:345:HOH:O	2.54	0.41
3:3:73:VAL:HA	3:3:74:PRO:HD2	1.91	0.41
4:4:21:ILE:C	4:4:23:ASN:N	2.69	0.41
1:1:3:ASP:HB2	5:1:338:HOH:O	2.20	0.41
3:3:31:SER:O	3:3:32:THR:C	2.59	0.41
2:2:218:THR:HG22	2:2:219:GLN:N	2.36	0.41
2:2:134:PHE:CE1	2:2:181:GLN:HG2	2.56	0.41
2:2:32:ARG:CZ	2:2:111:ARG:NH1	2.84	0.41
1:1:245:CYS:HA	1:1:246:PRO:HD2	1.85	0.41
3:3:121:VAL:CG1	3:3:122:LYS:N	2.84	0.41
3:3:187:TRP:N	3:3:187:TRP:CE3	2.89	0.40
2:2:181:GLN:HE21	2:2:181:GLN:HB2	1.70	0.40
1:1:187:VAL:HA	1:1:188:PRO:HD3	1.85	0.40
1:1:104:PHE:HB3	1:1:105:PRO:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:151:PHE:CD1	2:2:151:PHE:N	2.85	0.40
1:1:58:TYR:HA	1:1:66:ASN:HD21	1.87	0.40
1:1:75:SER:HB2	1:1:91:VAL:O	2.21	0.40
3:3:64:TYR:C	3:3:66:TYR:N	2.74	0.40
3:3:36:TYR:CE2	3:3:37:MET:HG2	2.57	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	254/274 (93%)	222 (87%)	22 (9%)	10 (4%)	4 12
2	2	253/267 (95%)	221 (87%)	29 (12%)	3 (1%)	16 47
3	3	226/236 (96%)	197 (87%)	23 (10%)	6 (3%)	6 21
4	4	23/71 (32%)	16 (70%)	4 (17%)	3 (13%)	0 1
All	All	756/848 (89%)	656 (87%)	78 (10%)	22 (3%)	6 19

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	51	ASN
1	1	202	ASN
3	3	83	VAL
3	3	91	CYS
4	4	22	ILE
4	4	25	PHE
1	1	119	PRO
3	3	60	ASN
3	3	87	CYS
4	4	23	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	33	VAL
1	1	81	THR
1	1	189	TYR
2	2	86	HIS
2	2	164	PRO
2	2	218	THR
1	1	28	GLU
1	1	20	VAL
1	1	154	VAL
3	3	19	PRO
3	3	85	LEU
1	1	255	PRO

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	220/237 (93%)	206 (94%)	14 (6%)	22 52
2	2	211/223 (95%)	198 (94%)	13 (6%)	23 54
3	3	200/205 (98%)	183 (92%)	17 (8%)	13 36
4	4	22/53 (42%)	19 (86%)	3 (14%)	5 14
All	All	653/718 (91%)	606 (93%)	47 (7%)	18 45

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	51	ASN
1	1	54	SER
1	1	61	ASN
1	1	66	ASN
1	1	68	LEU
1	1	80	SER
1	1	82	SER
1	1	118	SER
1	1	158	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	173	MET
1	1	212	ASP
1	1	241	MET
1	1	242	LYS
1	1	247	ARG
2	2	12	ASP
2	2	38	GLU
2	2	69	SER
2	2	141	LYS
2	2	152	THR
2	2	153	MET
2	2	171	SER
2	2	181	GLN
2	2	183	GLN
2	2	195	ASN
2	2	197	ARG
2	2	218	THR
2	2	265	ILE
3	3	1	SER
3	3	3	ILE
3	3	18	ASN
3	3	26	TYR
3	3	30	ILE
3	3	35	ASP
3	3	42	SER
3	3	61	ASN
3	3	75	THR
3	3	88	SER
3	3	91	CYS
3	3	108	SER
3	3	144	MET
3	3	158	SER
3	3	178	SER
3	3	192	GLN
3	3	225	SER
4	4	23	ASN
4	4	24	ASN
4	4	27	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	50	GLN
1	1	61	ASN
1	1	66	ASN
1	1	103	ASN
2	2	25	ASN
2	2	79	HIS
2	2	86	HIS
2	2	161	GLN
2	2	183	GLN
2	2	195	ASN
2	2	250	GLN
2	2	261	HIS
3	3	18	ASN
3	3	56	ASN
3	3	60	ASN
3	3	61	ASN
3	3	82	GLN
3	3	145	GLN
3	3	170	HIS
3	3	205	ASN
4	4	23	ASN
4	4	24	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

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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