



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:51 PM UTC

PDB ID : 2X53 / pdb_00002x53
Title : Structure of the phage p2 baseplate in its activated conformation with Sr
Authors : Sciara, G.; Bebeacua, C.; Bron, P.; Tremblay, D.; Ortiz-Lombardia, M.;
Lichiere, J.; van Heel, M.; Campanacci, V.; Moineau, S.; Cambillau, C.
Deposited on : 2010-02-05
Resolution : 3.90 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

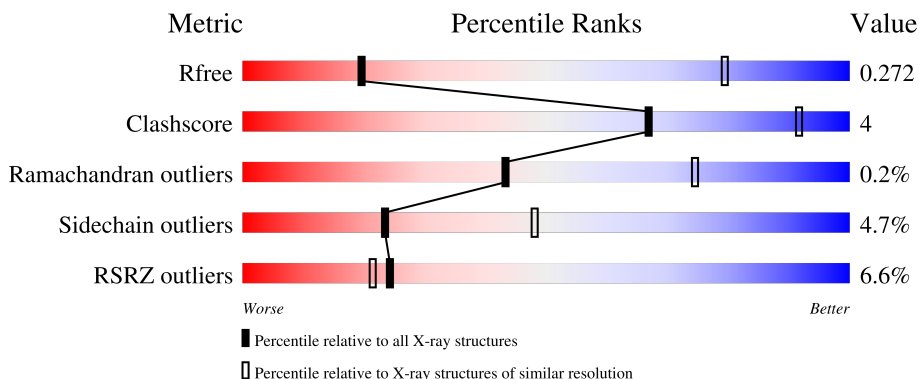
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	1	375	 5% 84% 13% ..
1	Y	375	 3% 84% 13% ...
1	Z	375	 5% 83% 14% ..
2	A	263	 2% 88% 11%
2	B	263	 3% 92% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	263	 2% 91% 9%
2	D	263	 5% 89% 10%
2	E	263	 13% 92% 8%
2	F	263	 11% 91% 9%
2	G	263	 8% 89% 10%
2	H	263	 17% 93% 7%
2	I	263	 16% 91% 9%
2	J	263	 5% 89% 10%
2	K	263	 2% 92% 7%
2	L	263	 7% 90% 10%
2	M	263	 6% 89% 10%
2	N	263	 6% 91% 9%
2	O	263	 7% 89% 11%
2	P	263	 9% 90% 10%
2	Q	263	 15% 92% 8%
2	R	263	 14% 89% 10%
3	S	298	 2% 77% 19%
3	T	298	 3% 76% 20% 5%
3	U	298	 4% 75% 22%
3	V	298	 3% 78% 19%
3	W	298	 4% 78% 18%
3	X	298	 5% 77% 19%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 59742 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 ORF16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	372	Total 3000	C 1918	N 493	O 581	S 8	0	0	0
1	Y	372	Total 3000	C 1918	N 493	O 581	S 8	0	0	0
1	Z	372	Total 3000	C 1918	N 493	O 581	S 8	0	0	0

- Molecule 2 is a protein called PUTATIVE RECEPTOR BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	B	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	C	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	D	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	E	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	F	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	G	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	H	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	I	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	J	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0
2	K	263	Total 2008	C 1260	N 346	O 396	S 6	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	M	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	N	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	O	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	P	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	Q	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			
2	R	263	Total	C	N	O	S	0	0	0
			2008	1260	346	396	6			

- Molecule 3 is a protein called ORF15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	T	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	U	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	V	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	W	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			
3	X	298	Total	C	N	O	S	0	0	0
			2432	1565	392	469	6			

- Molecule 4 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	S	1	Total	Sr	0	0
			1	1		
4	T	1	Total	Sr	0	0
			1	1		
4	U	1	Total	Sr	0	0
			1	1		
4	V	1	Total	Sr	0	0
			1	1		

Continued on next page...

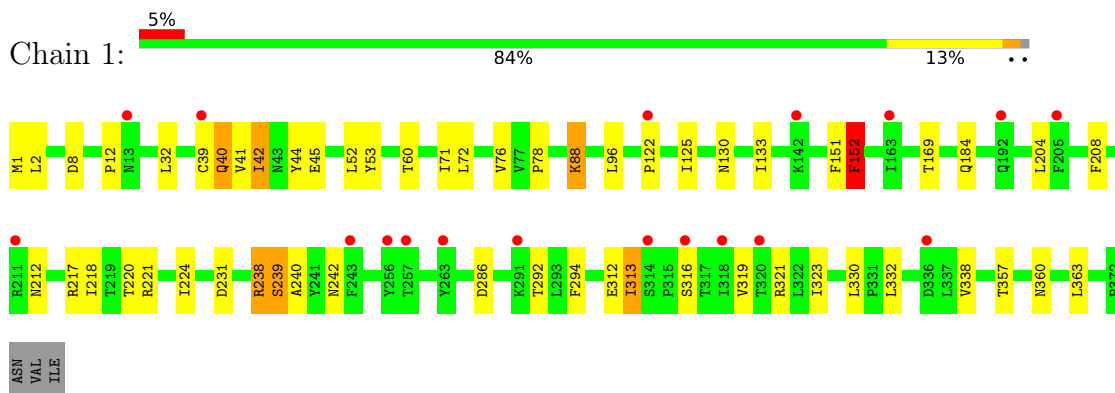
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	1	Total 1	Sr 1	0	0
4	X	1	Total 1	Sr 1	0	0

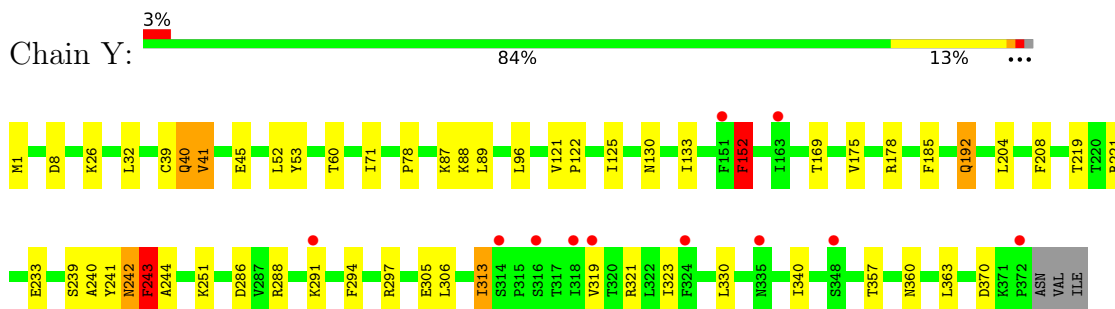
3 Residue-property plots [i](#)

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 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.

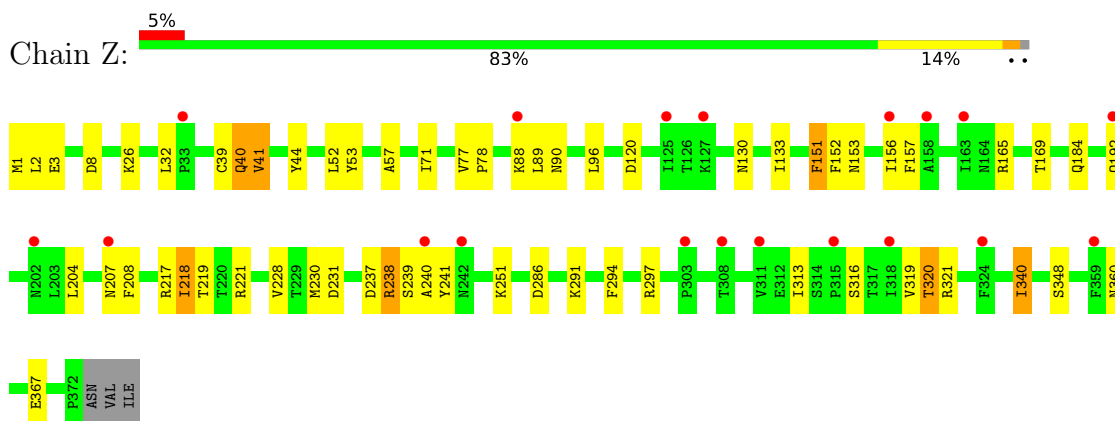
- Molecule 1: ORF16



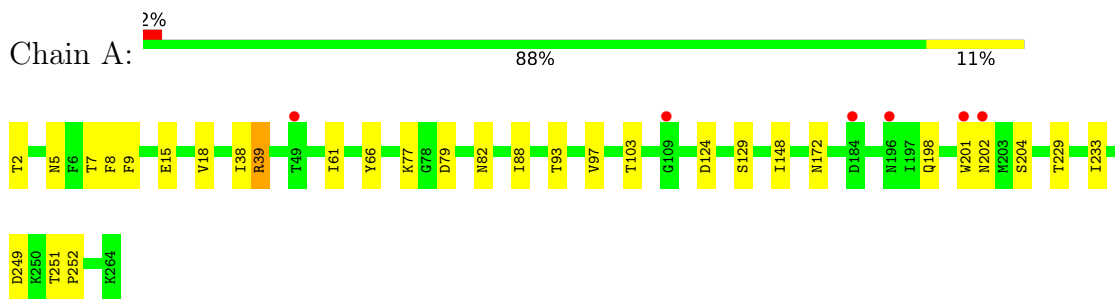
- Molecule 1: ORF16



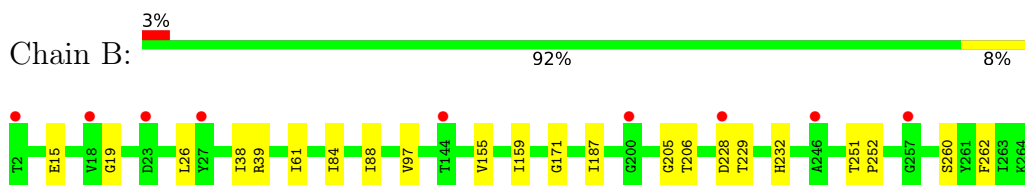
- Molecule 1: ORF16



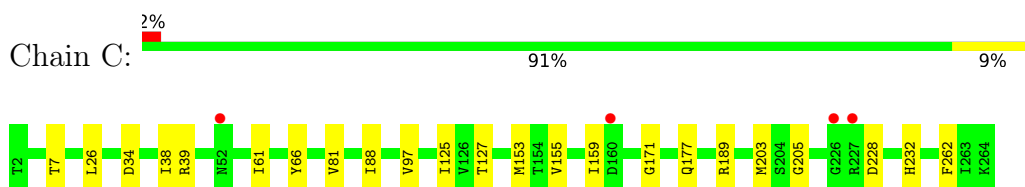
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



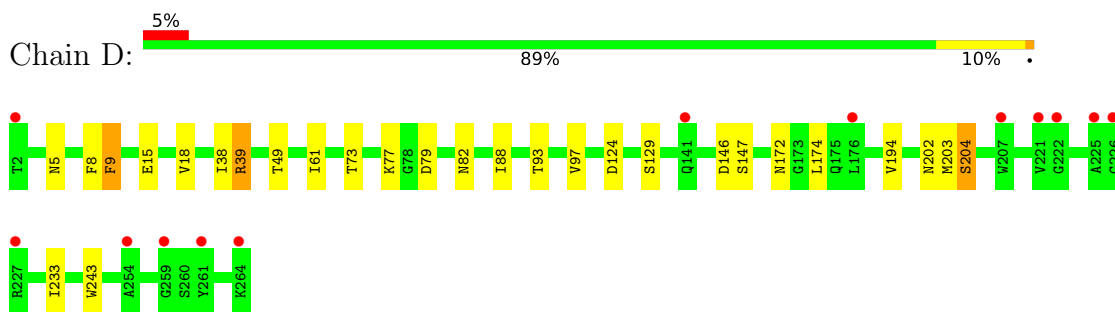
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



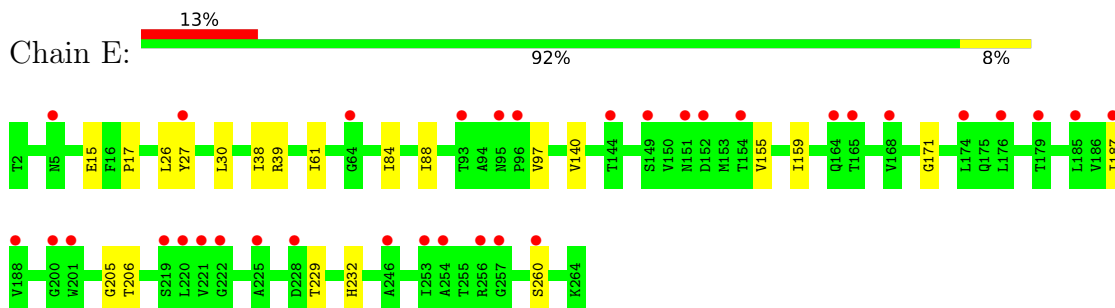
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



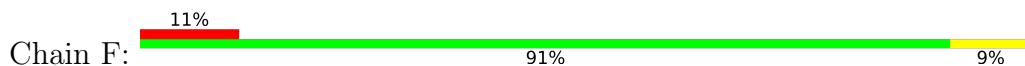
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

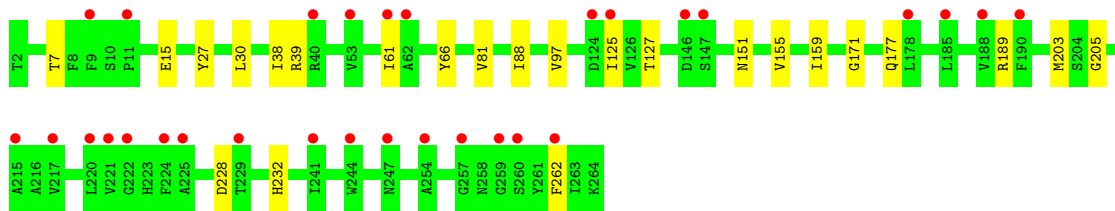


- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

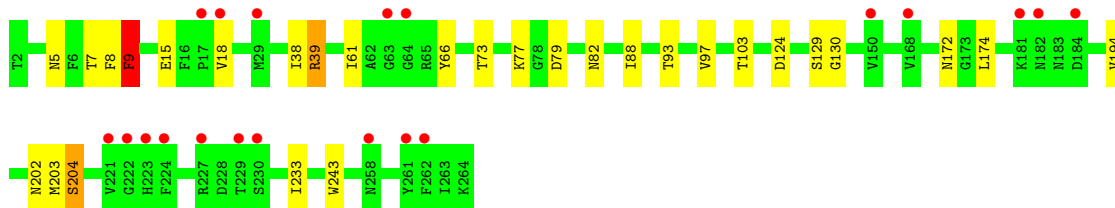
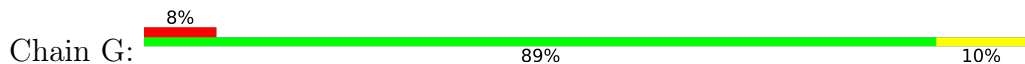


- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

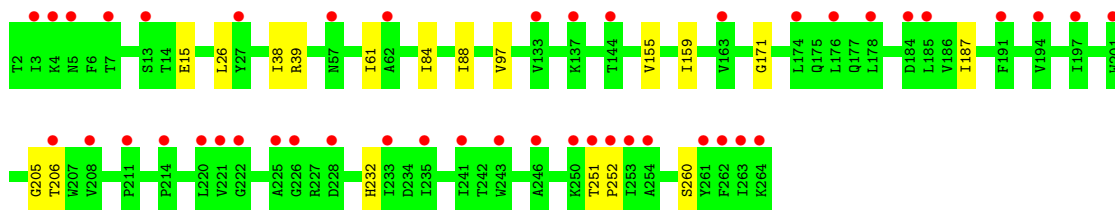
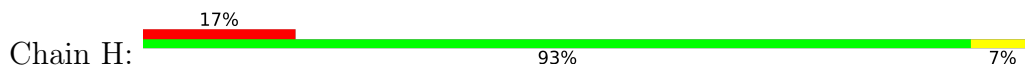




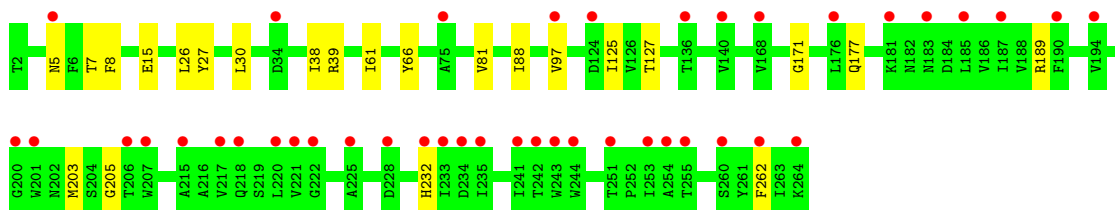
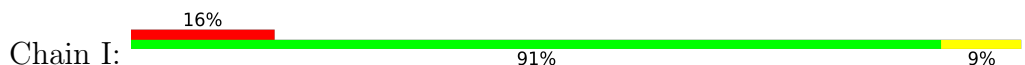
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



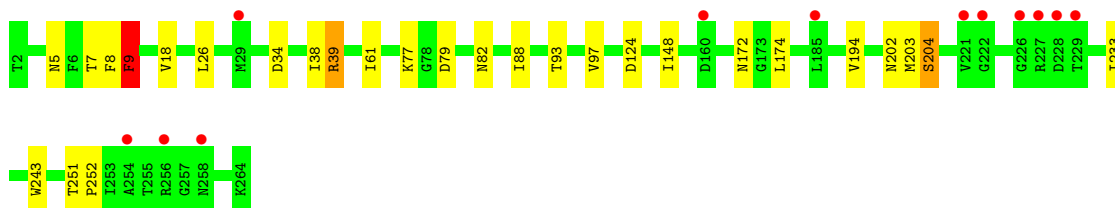
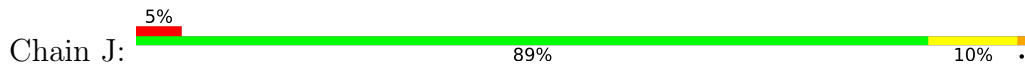
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



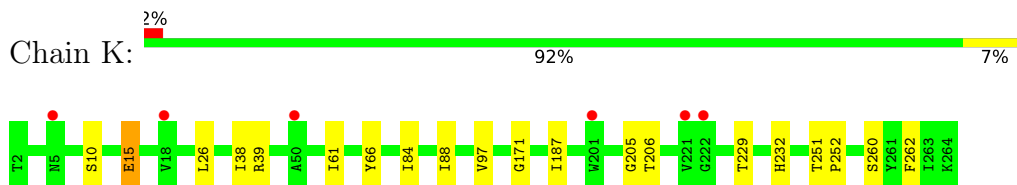
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



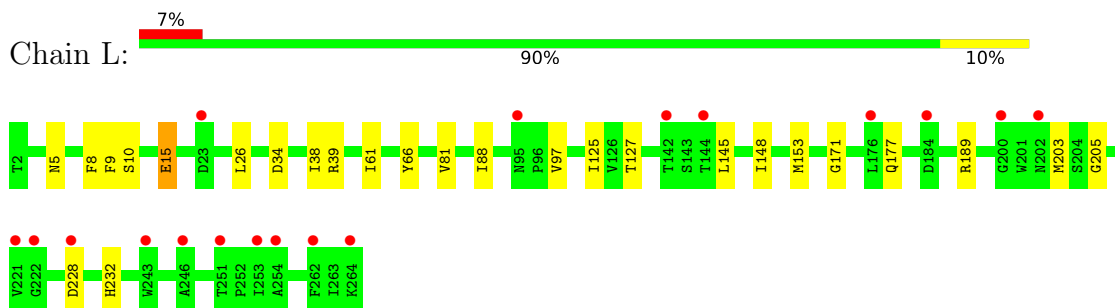
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



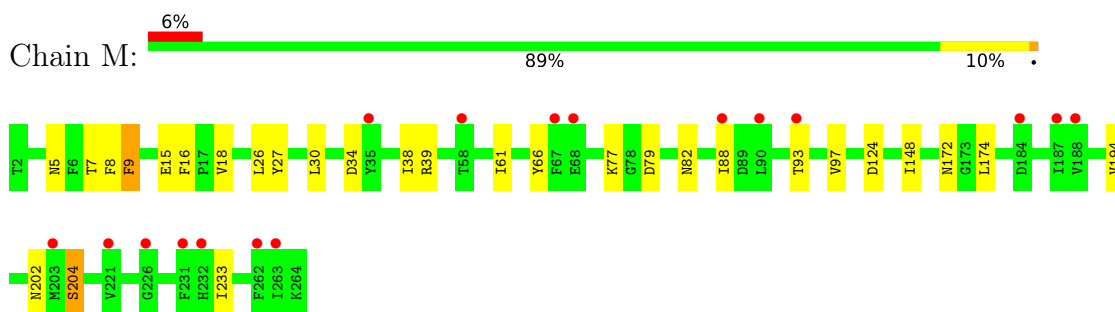
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



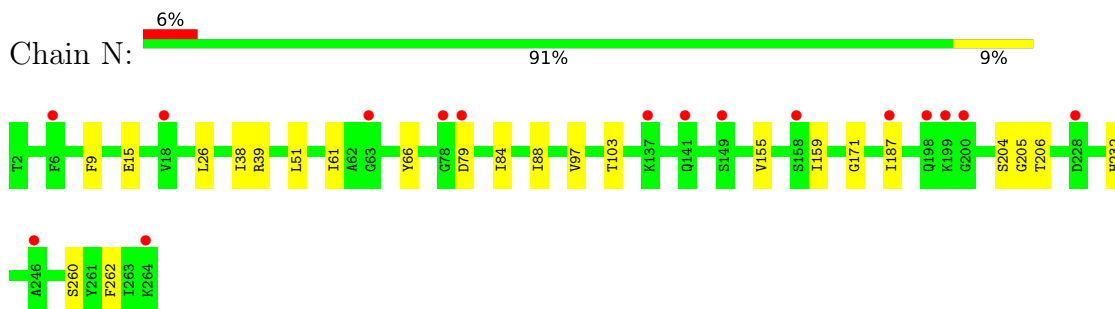
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



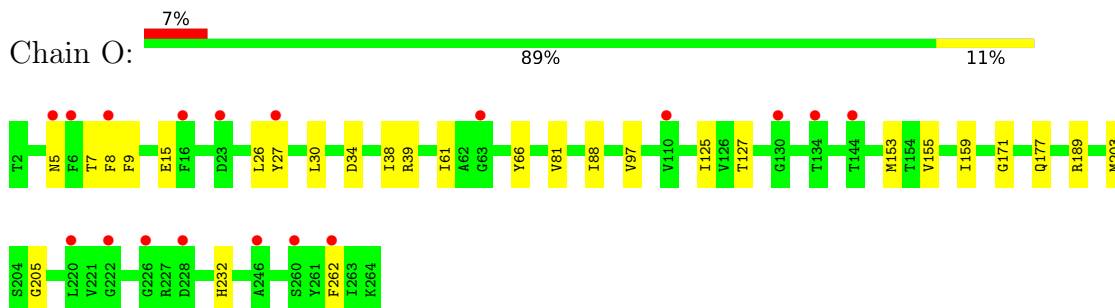
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



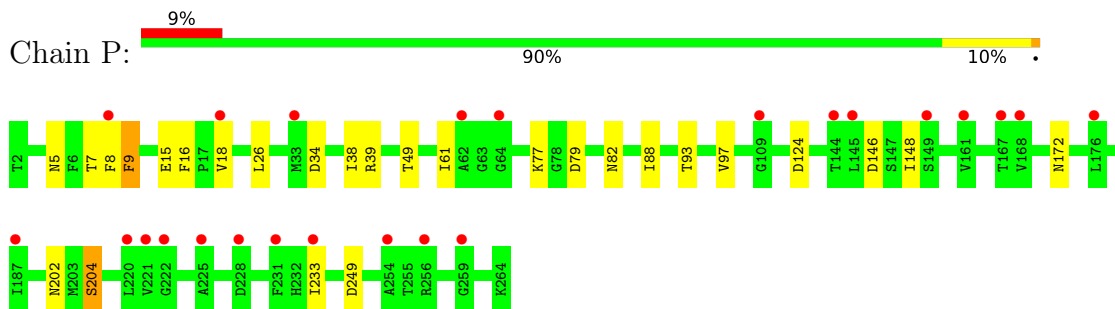
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



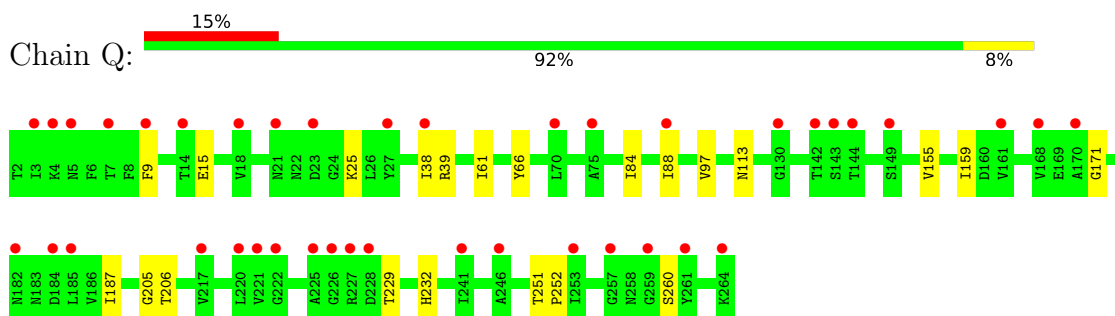
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



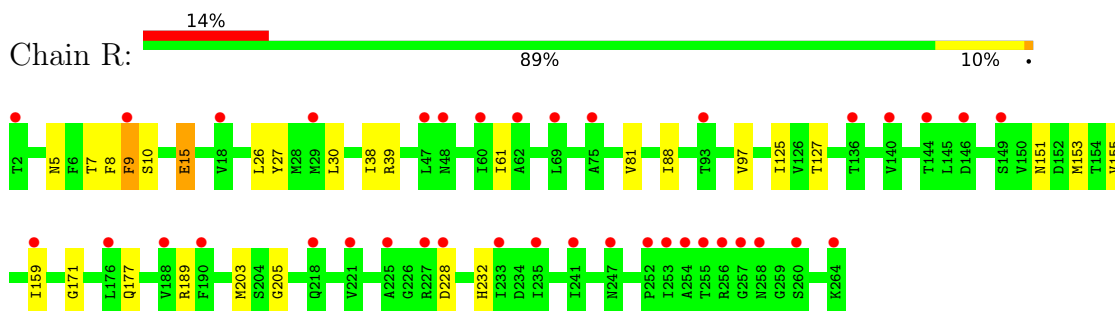
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



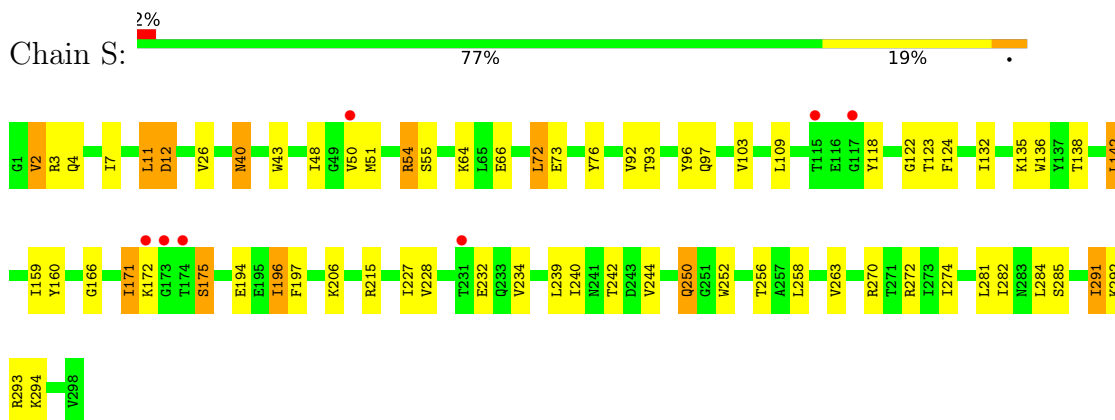
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



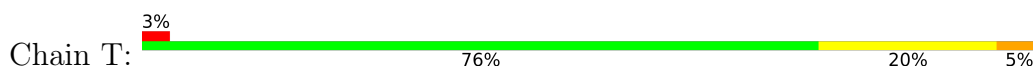
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

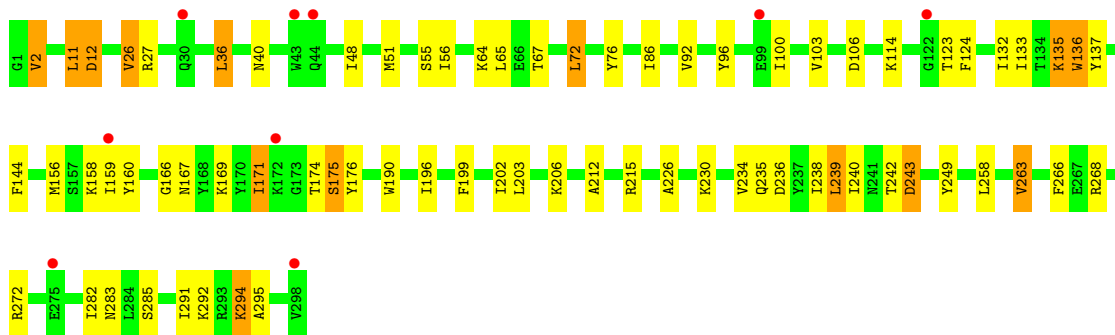


- Molecule 3: ORF15

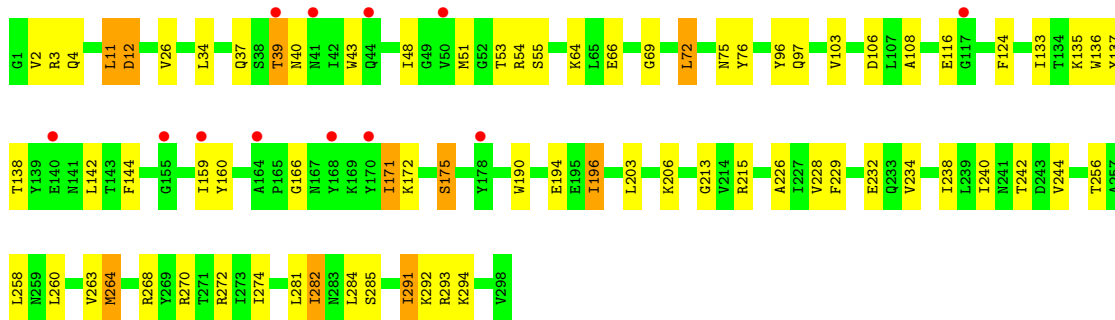
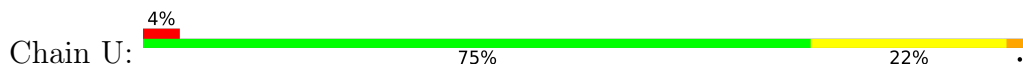


- Molecule 3: ORF15

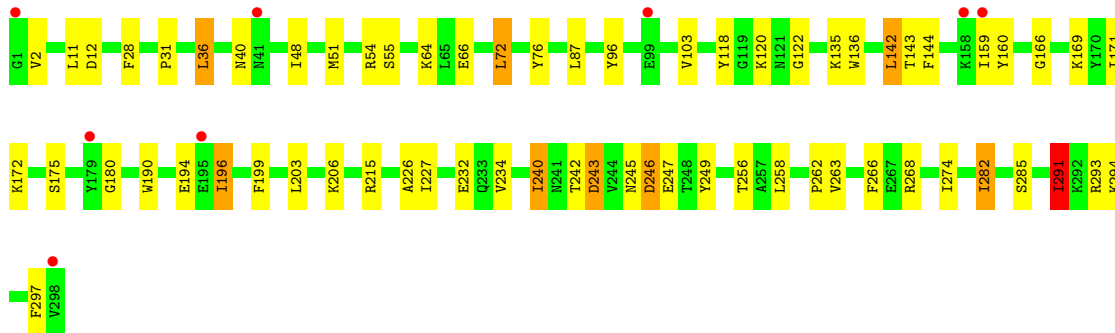
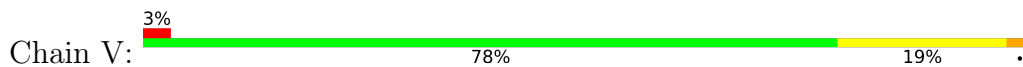




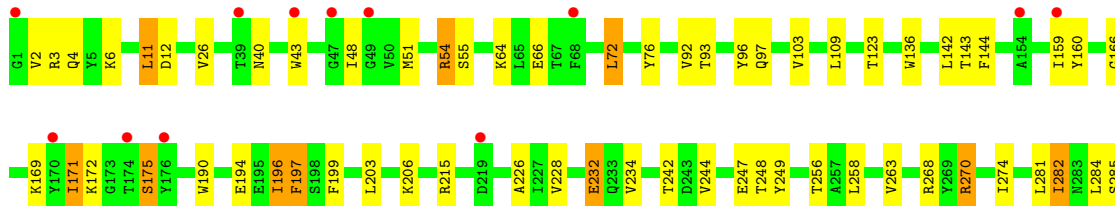
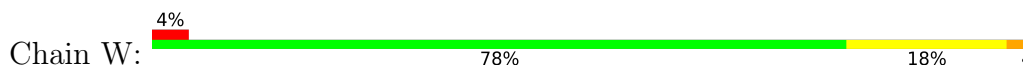
• Molecule 3: ORF15



• Molecule 3: ORF15

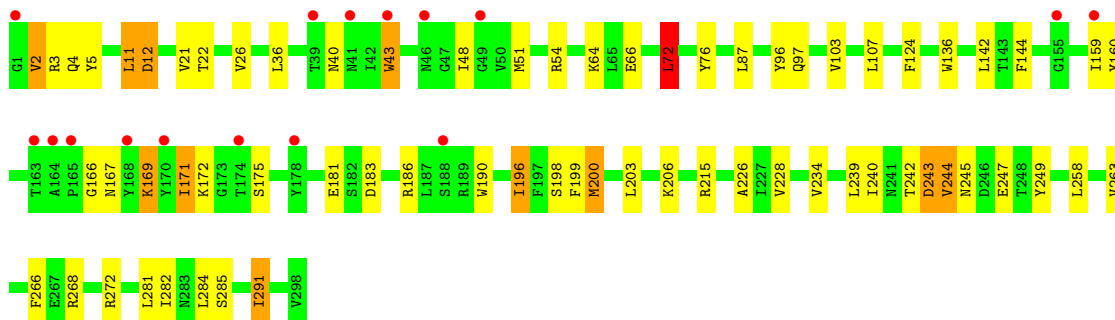
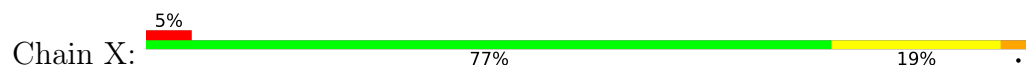


• Molecule 3: ORF15





- Molecule 3: ORF15



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	300.28Å 239.51Å 274.78Å 90.00° 124.36° 90.00°	Depositor
Resolution (Å)	39.31 – 3.90 39.31 – 3.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.31-3.90) 96.8 (39.31-3.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.87Å)	Xtrriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.229 , 0.242 0.260 , 0.272	Depositor DCC
R_{free} test set	4226 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	83.1	Xtrriage
Anisotropy	0.130	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 90.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	59742	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SR

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	0.72	0/3069	1.26	5/4175 (0.1%)
1	Y	0.72	0/3069	1.26	12/4175 (0.3%)
1	Z	0.71	0/3069	1.23	7/4175 (0.2%)
2	A	0.58	0/2048	1.07	4/2791 (0.1%)
2	B	0.69	0/2048	1.14	2/2791 (0.1%)
2	C	0.70	0/2048	1.16	4/2791 (0.1%)
2	D	0.57	0/2048	1.05	4/2791 (0.1%)
2	E	0.71	0/2048	1.15	1/2791 (0.0%)
2	F	0.72	0/2048	1.16	4/2791 (0.1%)
2	G	0.57	0/2048	1.05	5/2791 (0.2%)
2	H	0.71	0/2048	1.15	1/2791 (0.0%)
2	I	0.72	0/2048	1.16	4/2791 (0.1%)
2	J	0.62	0/2048	1.10	4/2791 (0.1%)
2	K	0.69	0/2048	1.15	2/2791 (0.1%)
2	L	0.71	0/2048	1.15	5/2791 (0.2%)
2	M	0.62	0/2048	1.11	4/2791 (0.1%)
2	N	0.69	0/2048	1.15	4/2791 (0.1%)
2	O	0.71	0/2048	1.16	6/2791 (0.2%)
2	P	0.62	0/2048	1.11	5/2791 (0.2%)
2	Q	0.71	0/2048	1.14	2/2791 (0.1%)
2	R	0.73	0/2048	1.16	4/2791 (0.1%)
3	S	0.62	0/2485	1.17	7/3356 (0.2%)
3	T	0.63	0/2485	1.20	8/3356 (0.2%)
3	U	0.63	0/2485	1.17	5/3356 (0.1%)
3	V	0.65	0/2485	1.17	3/3356 (0.1%)
3	W	0.63	0/2485	1.16	2/3356 (0.1%)
3	X	0.65	1/2485 (0.0%)	1.18	6/3356 (0.2%)
All	All	0.67	1/60981 (0.0%)	1.16	120/82899 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	22	THR	CA-C	6.80	1.61	1.53

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	Y	152	PHE	CA-CB-CG	12.00	125.80	113.80
1	1	152	PHE	CA-CB-CG	11.53	125.33	113.80
2	K	15	GLU	N-CA-C	7.53	119.18	110.97
3	W	12	ASP	CA-CB-CG	7.53	120.13	112.60
1	1	240	ALA	N-CA-C	6.94	121.91	113.17
3	U	124	PHE	CA-CB-CG	6.82	120.62	113.80
3	T	294	LYS	N-CA-C	6.70	118.65	110.41
3	X	12	ASP	CA-CB-CG	6.67	119.27	112.60
3	V	12	ASP	CA-CB-CG	6.62	119.22	112.60
3	T	12	ASP	CA-CB-CG	6.53	119.13	112.60
2	R	9	PHE	N-CA-C	6.48	120.38	109.76
3	S	12	ASP	CA-CB-CG	6.46	119.06	112.60
1	1	239	SER	N-CA-C	6.32	119.42	110.50
3	U	12	ASP	CA-CB-CG	6.18	118.78	112.60
2	A	15	GLU	N-CA-C	6.07	117.56	111.07
2	P	249	ASP	CA-C-N	6.01	128.62	120.38
2	P	249	ASP	C-N-CA	6.01	128.62	120.38
1	Y	242	ASN	N-CA-C	6.00	118.61	111.71
1	Y	240	ALA	N-CA-C	5.89	120.59	113.17
2	D	15	GLU	N-CA-C	5.89	117.37	111.07
2	P	15	GLU	N-CA-C	5.88	117.36	111.07
2	R	203	MET	CA-C-N	5.83	129.56	120.82
2	R	203	MET	C-N-CA	5.83	129.56	120.82
1	Y	219	THR	CB-CA-C	5.81	119.81	110.16
1	Y	243	PHE	CA-CB-CG	5.80	119.60	113.80
1	Z	151	PHE	CA-CB-CG	5.80	119.60	113.80
2	C	203	MET	CA-C-N	5.78	129.49	120.82
2	C	203	MET	C-N-CA	5.78	129.49	120.82
3	T	2	VAL	CA-C-N	5.78	129.08	120.87
3	T	2	VAL	C-N-CA	5.78	129.08	120.87
2	I	203	MET	CA-C-N	5.77	129.48	120.82
2	I	203	MET	C-N-CA	5.77	129.48	120.82
2	O	203	MET	CA-C-N	5.77	129.47	120.82
2	O	203	MET	C-N-CA	5.77	129.47	120.82
2	O	15	GLU	N-CA-C	5.74	118.03	111.02
2	L	203	MET	CA-C-N	5.74	129.43	120.82
2	L	203	MET	C-N-CA	5.74	129.43	120.82
3	S	2	VAL	CA-C-N	5.73	129.01	120.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	2	VAL	C-N-CA	5.73	129.01	120.87
2	F	203	MET	CA-C-N	5.72	129.40	120.82
2	F	203	MET	C-N-CA	5.72	129.40	120.82
3	S	197	PHE	CA-CB-CG	5.72	119.52	113.80
1	Z	240	ALA	N-CA-C	5.72	120.38	113.17
2	L	15	GLU	N-CA-C	5.68	117.95	111.02
1	Y	244	ALA	N-CA-C	5.66	118.18	109.07
3	X	2	VAL	CA-C-N	5.65	128.89	120.87
3	X	2	VAL	C-N-CA	5.65	128.89	120.87
2	L	9	PHE	N-CA-C	5.64	119.02	109.76
2	M	204	SER	N-CA-C	5.64	119.90	113.19
2	P	204	SER	N-CA-C	5.63	119.89	113.19
2	J	204	SER	N-CA-C	5.62	119.88	113.19
2	Q	15	GLU	N-CA-C	5.59	117.84	111.02
3	U	39	THR	N-CA-C	-5.58	100.08	109.07
2	B	15	GLU	N-CA-C	5.58	117.83	111.02
2	G	204	SER	N-CA-C	5.57	119.82	113.19
2	J	9	PHE	CA-CB-CG	5.57	119.37	113.80
2	G	9	PHE	CA-CB-CG	5.56	119.36	113.80
3	U	264	MET	N-CA-C	5.56	117.72	110.43
2	M	15	GLU	N-CA-C	5.56	117.78	111.11
1	Z	219	THR	CB-CA-C	5.55	119.68	110.74
2	G	15	GLU	N-CA-C	5.54	117.78	111.02
2	D	204	SER	N-CA-C	5.53	119.77	113.19
1	1	151	PHE	CA-CB-CG	5.52	119.32	113.80
2	H	15	GLU	N-CA-C	5.47	117.70	111.02
2	M	34	ASP	CA-CB-CG	5.47	118.07	112.60
2	E	15	GLU	N-CA-C	5.42	117.64	111.02
1	Y	239	SER	N-CA-C	5.41	117.87	110.24
3	S	124	PHE	CA-CB-CG	5.38	119.18	113.80
3	X	72	LEU	CA-C-N	5.38	127.43	120.44
3	X	72	LEU	C-N-CA	5.38	127.43	120.44
1	1	44	TYR	N-CA-C	5.36	118.47	109.95
3	T	124	PHE	CA-CB-CG	5.36	119.16	113.80
1	Z	228	VAL	N-CA-C	5.34	115.97	109.30
2	D	39	ARG	N-CA-C	-5.28	100.30	108.90
3	T	27	ARG	N-CA-C	5.28	118.00	109.40
2	R	15	GLU	N-CA-C	5.27	117.45	111.02
1	Z	44	TYR	N-CA-C	5.23	118.11	109.85
1	Y	152	PHE	N-CA-C	5.23	117.94	109.06
2	F	15	GLU	N-CA-C	5.22	117.39	111.02
2	O	9	PHE	N-CA-C	5.21	118.72	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	249	ASP	CA-CB-CG	5.21	117.81	112.60
3	X	124	PHE	CA-CB-CG	5.20	119.00	113.80
3	S	40	ASN	N-CA-C	5.20	119.47	113.18
2	G	39	ARG	N-CA-C	-5.19	100.44	108.90
2	N	15	GLU	N-CA-C	5.19	117.35	111.02
2	G	129	SER	N-CA-C	-5.19	100.98	109.80
1	Z	239	SER	N-CA-C	5.18	117.74	110.23
2	A	39	ARG	N-CA-C	-5.18	100.46	108.90
2	Q	9	PHE	CA-CB-CG	5.17	118.97	113.80
3	T	294	LYS	CA-C-N	5.17	129.26	121.40
3	T	294	LYS	C-N-CA	5.17	129.26	121.40
3	S	250	GLN	N-CA-C	5.17	117.32	108.90
3	U	291	ILE	N-CA-C	5.16	115.73	108.36
2	C	262	PHE	CA-CB-CG	5.15	118.95	113.80
2	M	9	PHE	CA-CB-CG	5.15	118.95	113.80
1	Y	305	GLU	CA-C-N	5.14	127.17	120.28
1	Y	305	GLU	C-N-CA	5.14	127.17	120.28
2	K	262	PHE	CA-CB-CG	5.12	118.92	113.80
1	Z	340	ILE	N-CA-C	5.10	115.65	108.36
2	A	129	SER	N-CA-C	-5.09	101.14	109.80
2	J	34	ASP	CA-CB-CG	5.09	117.69	112.60
3	W	197	PHE	CA-CB-CG	5.09	118.89	113.80
2	I	262	PHE	CA-CB-CG	5.09	118.89	113.80
2	D	129	SER	N-CA-C	-5.08	101.17	109.80
1	Y	370	ASP	CA-C-N	5.07	126.07	119.78
1	Y	370	ASP	C-N-CA	5.07	126.07	119.78
2	B	262	PHE	CA-CB-CG	5.07	118.87	113.80
2	P	34	ASP	CA-CB-CG	5.07	117.67	112.60
2	O	262	PHE	CA-CB-CG	5.06	118.86	113.80
2	I	15	GLU	N-CA-C	5.04	117.16	111.02
2	L	34	ASP	CA-CB-CG	5.04	117.64	112.60
2	N	9	PHE	CA-CB-CG	5.03	118.83	113.80
3	V	28	PHE	CA-CB-CG	5.02	118.82	113.80
2	C	34	ASP	CA-CB-CG	5.02	117.62	112.60
3	V	291	ILE	N-CA-C	5.02	115.53	108.36
2	F	262	PHE	CA-CB-CG	5.01	118.81	113.80
2	J	39	ARG	N-CA-C	-5.01	100.73	108.90
2	O	34	ASP	CA-CB-CG	5.01	117.61	112.60
2	N	204	SER	N-CA-C	5.01	116.74	111.28
2	N	262	PHE	CA-CB-CG	5.01	118.81	113.80

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	3000	0	2956	37	0
1	Y	3000	0	2956	26	0
1	Z	3000	0	2956	33	0
2	A	2008	0	1971	13	0
2	B	2008	0	1971	10	0
2	C	2008	0	1971	10	0
2	D	2008	0	1971	14	0
2	E	2008	0	1971	10	0
2	F	2008	0	1971	10	0
2	G	2008	0	1971	16	0
2	H	2008	0	1971	7	0
2	I	2008	0	1971	9	0
2	J	2008	0	1971	13	0
2	K	2008	0	1971	9	0
2	L	2008	0	1971	11	0
2	M	2008	0	1971	13	0
2	N	2008	0	1971	11	0
2	O	2008	0	1971	11	0
2	P	2008	0	1971	14	0
2	Q	2008	0	1971	10	0
2	R	2008	0	1971	16	0
3	S	2432	0	2394	38	0
3	T	2432	0	2394	38	0
3	U	2432	0	2394	36	0
3	V	2432	0	2394	29	0
3	W	2432	0	2394	25	0
3	X	2432	0	2394	44	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
4	U	1	0	0	0	0
4	V	1	0	0	0	0
4	W	1	0	0	0	0
4	X	1	0	0	0	0
All	All	59742	0	58710	441	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 4.

All (441) 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)
1:1:78:PRO:HG3	2:N:103:THR:HB	1.31	1.08
2:G:103:THR:HB	1:Z:78:PRO:HG3	1.41	1.00
3:S:242:THR:CG2	3:S:272:ARG:HG3	1.90	1.00
2:A:103:THR:HB	1:Y:78:PRO:HG3	1.48	0.94
1:1:42:ILE:HB	3:X:43:TRP:HZ2	1.33	0.94
1:1:42:ILE:HB	3:X:43:TRP:CZ2	2.07	0.90
2:R:9:PHE:CE2	3:X:181:GLU:HG3	2.08	0.89
2:R:9:PHE:CZ	3:X:181:GLU:HG3	2.13	0.84
1:1:239:SER:HB2	1:1:312:GLU:O	1.81	0.81
3:S:142:LEU:HD12	3:S:291:ILE:HD12	1.65	0.77
3:S:242:THR:HG22	3:S:272:ARG:HG3	1.64	0.76
3:U:242:THR:CG2	3:U:272:ARG:HG3	2.16	0.76
1:Y:169:THR:HG21	1:Z:294:PHE:CE2	2.26	0.71
2:A:77:LYS:H	2:A:82:ASN:HD21	1.39	0.70
2:P:77:LYS:H	2:P:82:ASN:HD21	1.41	0.69
3:S:242:THR:HG22	3:S:272:ARG:CG	2.22	0.69
3:S:250:GLN:HE21	3:S:252:TRP:HE1	1.42	0.68
2:D:77:LYS:H	2:D:82:ASN:HD21	1.42	0.68
2:G:77:LYS:H	2:G:82:ASN:HD21	1.42	0.68
3:W:142:LEU:HG	3:W:291:ILE:HD12	1.77	0.67
1:1:294:PHE:CE2	1:Z:169:THR:HG21	2.30	0.66
2:M:77:LYS:H	2:M:82:ASN:HD21	1.42	0.66
1:Z:238:ARG:HG3	1:Z:316:SER:HA	1.78	0.65
1:Y:243:PHE:HA	1:Y:313:ILE:HD11	1.79	0.65
2:J:77:LYS:H	2:J:82:ASN:HD21	1.41	0.65
1:Z:89:LEU:HD22	1:Z:192:GLN:HG3	1.79	0.64
1:1:294:PHE:HE2	1:Z:169:THR:HG21	1.62	0.64
2:R:9:PHE:HE2	3:X:181:GLU:HG3	1.63	0.63
3:S:250:GLN:NE2	3:S:252:TRP:HE1	1.96	0.63
3:V:247:GLU:OE1	3:V:249:TYR:HE2	1.81	0.62
3:X:11:LEU:HD23	3:X:12:ASP:H	1.64	0.62
1:Y:152:PHE:HB2	1:Y:208:PHE:HB2	1.80	0.62
3:S:215:ARG:HB3	3:S:282:ILE:HD11	1.82	0.62
1:1:152:PHE:HB2	1:1:208:PHE:HB2	1.80	0.62
1:Y:241:TYR:HB2	1:Y:291:LYS:HD2	1.81	0.61
3:W:215:ARG:HB3	3:W:282:ILE:HD11	1.83	0.61
3:X:247:GLU:OE1	3:X:249:TYR:HE2	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:90:ASN:HD22	1:Z:192:GLN:NE2	1.99	0.61
3:U:137:TYR:HD1	3:U:292:LYS:HB2	1.66	0.60
3:T:235:GLN:HE22	3:T:258:LEU:HD12	1.67	0.60
3:X:215:ARG:HB3	3:X:282:ILE:HD11	1.84	0.60
3:U:215:ARG:HB3	3:U:282:ILE:HD11	1.83	0.59
3:S:206:LYS:HG3	3:S:285:SER:HB3	1.84	0.59
3:U:116:GLU:HB2	3:V:31:PRO:HD2	1.85	0.59
2:G:103:THR:CB	1:Z:78:PRO:HG3	2.25	0.59
3:X:12:ASP:HB2	3:X:200:MET:HG3	1.84	0.59
3:S:196:ILE:HG13	3:S:274:ILE:HB	1.85	0.59
1:Y:243:PHE:CD1	1:Y:243:PHE:C	2.80	0.59
3:U:238:ILE:HG22	3:U:240:ILE:HG23	1.85	0.59
3:X:199:PHE:CE1	3:X:242:THR:HG21	2.37	0.59
2:O:88:ILE:HG12	2:O:97:VAL:HG22	1.86	0.58
2:R:88:ILE:HG12	2:R:97:VAL:HG22	1.85	0.58
3:V:247:GLU:OE1	3:V:249:TYR:CE2	2.56	0.58
1:Z:153:ASN:HB3	1:Z:156:ILE:HG12	1.85	0.58
2:I:88:ILE:HG12	2:I:97:VAL:HG22	1.85	0.58
3:X:266:PHE:HB3	1:Y:221:ARG:HB2	1.85	0.58
3:V:226:ALA:HB3	3:V:268:ARG:HB3	1.85	0.58
2:F:88:ILE:HG12	2:F:97:VAL:HG22	1.86	0.58
1:Z:41:VAL:HG23	1:Z:57:ALA:HB1	1.85	0.58
3:V:171:ILE:HG22	3:V:172:LYS:H	1.68	0.58
3:X:206:LYS:HG3	3:X:285:SER:HB3	1.86	0.58
2:L:88:ILE:HG12	2:L:97:VAL:HG22	1.86	0.57
3:U:242:THR:HG23	3:U:272:ARG:HG3	1.87	0.57
3:V:206:LYS:HG3	3:V:285:SER:HB3	1.87	0.57
3:X:199:PHE:N	3:X:242:THR:OG1	2.33	0.57
1:1:41:VAL:HG11	1:1:71:ILE:HG12	1.87	0.56
3:T:240:ILE:HD12	3:T:240:ILE:O	2.06	0.56
2:K:10:SER:HA	2:K:15:GLU:HB2	1.88	0.56
3:W:206:LYS:HG3	3:W:285:SER:HB3	1.87	0.56
2:C:88:ILE:HG12	2:C:97:VAL:HG22	1.86	0.56
2:B:187:ILE:HG12	2:B:260:SER:HB3	1.88	0.56
1:Z:41:VAL:HG11	1:Z:71:ILE:HG12	1.88	0.56
3:U:196:ILE:HG22	3:U:293:ARG:HD3	1.87	0.56
3:X:240:ILE:HD12	3:X:240:ILE:O	2.07	0.55
3:U:240:ILE:HD12	3:U:240:ILE:O	2.05	0.55
2:M:26:LEU:HD13	2:N:66:TYR:HB2	1.88	0.55
3:S:160:TYR:HB3	3:S:166:GLY:HA3	1.89	0.55
3:T:160:TYR:HB3	3:T:166:GLY:HA3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:187:ILE:HG12	2:E:260:SER:HB3	1.88	0.55
2:N:88:ILE:HG12	2:N:97:VAL:HG22	1.89	0.55
3:V:240:ILE:C	3:V:240:ILE:HD12	2.32	0.55
3:X:247:GLU:OE1	3:X:249:TYR:CE2	2.59	0.55
3:T:243:ASP:C	3:T:243:ASP:OD1	2.50	0.55
3:U:108:ALA:HB2	3:U:133:ILE:HD11	1.89	0.55
2:B:155:VAL:HG21	2:B:159:ILE:HD11	1.88	0.55
1:1:221:ARG:HB2	3:V:266:PHE:HB3	1.87	0.55
2:B:88:ILE:HG12	2:B:97:VAL:HG22	1.88	0.55
2:E:88:ILE:HG12	2:E:97:VAL:HG22	1.89	0.55
2:H:187:ILE:HG12	2:H:260:SER:HB3	1.88	0.55
2:P:5:ASN:HB3	2:P:8:PHE:CD1	2.42	0.55
3:X:40:ASN:HB3	3:X:51:MET:HE3	1.89	0.55
1:1:238:ARG:HG3	1:1:316:SER:HA	1.89	0.54
2:Q:187:ILE:HG12	2:Q:260:SER:HB3	1.88	0.54
2:Q:88:ILE:HG12	2:Q:97:VAL:HG22	1.89	0.54
3:S:11:LEU:O	3:S:12:ASP:CG	2.51	0.54
3:T:106:ASP:O	3:T:133:ILE:HB	2.08	0.54
2:K:88:ILE:HG12	2:K:97:VAL:HG22	1.89	0.54
2:N:187:ILE:HG12	2:N:260:SER:HB3	1.88	0.54
2:H:88:ILE:HG12	2:H:97:VAL:HG22	1.89	0.54
3:S:244:VAL:HG11	1:Y:1:MET:HE1	1.90	0.54
3:X:167:ASN:ND2	3:X:169:LYS:HE3	2.23	0.54
2:K:187:ILE:HG12	2:K:260:SER:HB3	1.89	0.54
2:D:9:PHE:HA	3:T:160:TYR:HB2	1.89	0.53
3:V:142:LEU:HG	3:V:291:ILE:HD12	1.90	0.53
3:X:226:ALA:HB3	3:X:268:ARG:HB3	1.89	0.53
1:Z:237:ASP:C	1:Z:238:ARG:HG2	2.33	0.53
2:P:88:ILE:HG12	2:P:97:VAL:HG22	1.91	0.53
3:U:160:TYR:HB3	3:U:166:GLY:HA3	1.89	0.53
2:P:26:LEU:HD13	2:Q:66:TYR:HB2	1.91	0.53
3:T:215:ARG:HB3	3:T:282:ILE:HD11	1.90	0.53
3:X:183:ASP:O	3:X:186:ARG:HG3	2.09	0.53
3:T:230:LYS:HG3	3:T:263:VAL:HG22	1.91	0.53
1:1:45:GLU:HA	1:1:357:THR:HG22	1.91	0.53
2:L:145:LEU:HD13	2:L:148:ILE:HD11	1.91	0.53
3:S:239:LEU:C	3:S:239:LEU:HD23	2.34	0.53
2:Q:25:LYS:HE2	2:Q:113:ASN:HB3	1.91	0.52
3:W:196:ILE:HG13	3:W:274:ILE:HB	1.90	0.52
3:X:160:TYR:HB3	3:X:166:GLY:HA3	1.92	0.52
2:M:88:ILE:HG12	2:M:97:VAL:HG22	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:88:ILE:HG12	2:G:97:VAL:HG22	1.90	0.52
1:1:42:ILE:CB	3:X:43:TRP:HZ2	2.14	0.52
2:G:73:THR:HG21	3:T:258:LEU:HD21	1.92	0.52
3:T:132:ILE:HD13	3:T:135:LYS:HG3	1.92	0.52
3:T:206:LYS:HG3	3:T:285:SER:HB3	1.91	0.52
3:V:243:ASP:C	3:V:243:ASP:OD1	2.52	0.52
3:X:144:PHE:HB3	3:X:190:TRP:CE2	2.45	0.52
1:Y:89:LEU:HD22	1:Y:192:GLN:HG3	1.92	0.52
2:J:88:ILE:HG12	2:J:97:VAL:HG22	1.90	0.52
2:A:5:ASN:HB3	2:A:8:PHE:CD1	2.44	0.52
3:W:226:ALA:HB3	3:W:268:ARG:HB3	1.92	0.52
1:Z:241:TYR:HB2	1:Z:291:LYS:HD2	1.91	0.52
2:D:5:ASN:HB3	2:D:8:PHE:CD1	2.44	0.52
3:U:11:LEU:O	3:U:12:ASP:CG	2.52	0.52
1:Y:32:LEU:HD11	1:Y:204:LEU:HB2	1.92	0.52
3:S:50:VAL:HG22	3:X:244:VAL:HG21	1.92	0.51
2:A:88:ILE:HG12	2:A:97:VAL:HG22	1.92	0.51
2:G:103:THR:HB	1:Z:78:PRO:CG	2.29	0.51
3:W:160:TYR:HB3	3:W:166:GLY:HA3	1.92	0.51
2:L:177:GLN:HB3	2:L:189:ARG:HB2	1.93	0.51
3:S:4:GLN:HB2	3:S:97:GLN:HB3	1.93	0.51
2:I:177:GLN:HB3	2:I:189:ARG:HB2	1.93	0.51
3:T:199:PHE:H	3:T:242:THR:HG1	1.57	0.51
3:U:138:THR:O	3:U:292:LYS:HA	2.11	0.51
2:C:177:GLN:HB3	2:C:189:ARG:HB2	1.93	0.50
2:O:177:GLN:HB3	2:O:189:ARG:HB2	1.93	0.50
3:T:199:PHE:N	3:T:242:THR:OG1	2.39	0.50
2:A:148:ILE:HB	2:C:153:MET:HG3	1.92	0.50
3:V:196:ILE:HG13	3:V:274:ILE:HB	1.93	0.50
1:Z:157:PHE:HE2	1:Z:208:PHE:HB3	1.76	0.50
2:A:172:ASN:HD21	2:A:204:SER:H	1.60	0.50
2:J:26:LEU:HD13	2:K:66:TYR:HB2	1.94	0.50
2:P:5:ASN:O	2:P:16:PHE:HB3	2.11	0.50
1:1:32:LEU:HD11	1:1:204:LEU:HB2	1.93	0.50
2:O:171:GLY:HA3	2:O:205:GLY:H	1.77	0.50
2:L:171:GLY:HA3	2:L:205:GLY:H	1.77	0.50
2:R:171:GLY:HA3	2:R:205:GLY:H	1.77	0.50
3:T:36:LEU:HD22	3:T:56:ILE:HD11	1.94	0.50
3:T:156:MET:HE3	3:T:174:THR:HG22	1.94	0.50
3:V:96:TYR:HB3	3:V:103:VAL:HG23	1.94	0.50
2:D:88:ILE:HG12	2:D:97:VAL:HG22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:171:GLY:HA3	2:F:205:GLY:H	1.77	0.50
2:Q:39:ARG:HB2	2:Q:61:ILE:HB	1.94	0.50
3:X:167:ASN:HD22	3:X:169:LYS:HE3	1.76	0.50
3:S:171:ILE:HG22	3:S:172:LYS:H	1.76	0.49
3:U:196:ILE:HG13	3:U:274:ILE:HB	1.94	0.49
3:U:281:LEU:HB3	3:U:284:LEU:HD12	1.92	0.49
3:W:4:GLN:HB2	3:W:97:GLN:HB3	1.94	0.49
2:G:130:GLY:HA3	1:Z:218:ILE:HG23	1.94	0.49
2:P:49:THR:HG22	3:W:232:GLU:HB2	1.94	0.49
2:R:177:GLN:HB3	2:R:189:ARG:HB2	1.93	0.49
3:X:199:PHE:CZ	3:X:242:THR:HG21	2.47	0.49
1:1:122:PRO:HD2	1:1:125:ILE:HD12	1.94	0.49
2:F:177:GLN:HB3	2:F:189:ARG:HB2	1.93	0.49
2:J:5:ASN:HB3	2:J:8:PHE:CD1	2.47	0.49
1:Y:39:CYS:HB2	1:Y:60:THR:OG1	2.12	0.49
3:T:238:ILE:HG22	3:T:240:ILE:HG23	1.94	0.49
2:K:39:ARG:HB2	2:K:61:ILE:HB	1.94	0.49
3:U:229:PHE:CD1	3:U:264:MET:HB3	2.48	0.49
3:X:171:ILE:HG22	3:X:172:LYS:H	1.77	0.49
1:1:218:ILE:HB	1:1:338:VAL:HG12	1.95	0.49
2:H:39:ARG:HB2	2:H:61:ILE:HB	1.94	0.49
1:1:76:VAL:HG11	1:1:88:LYS:HD2	1.94	0.49
2:C:171:GLY:HA3	2:C:205:GLY:H	1.77	0.49
1:1:184:GLN:HE22	1:1:217:ARG:HH22	1.61	0.49
1:1:242:ASN:O	1:1:313:ILE:HD12	2.12	0.49
2:I:171:GLY:HA3	2:I:205:GLY:H	1.77	0.49
2:N:39:ARG:HB2	2:N:61:ILE:HB	1.93	0.49
2:B:39:ARG:HB2	2:B:61:ILE:HB	1.95	0.49
1:Z:152:PHE:CB	1:Z:208:PHE:HB2	2.42	0.49
2:J:9:PHE:HB2	3:V:180:GLY:HA2	1.95	0.48
3:V:215:ARG:HB3	3:V:282:ILE:HD11	1.95	0.48
1:Y:233:GLU:HB2	1:Y:321:ARG:HH21	1.78	0.48
3:S:196:ILE:HG22	3:S:293:ARG:HD3	1.95	0.48
2:E:39:ARG:HB2	2:E:61:ILE:HB	1.94	0.48
2:I:27:TYR:HA	2:I:30:LEU:HD12	1.96	0.48
3:U:171:ILE:HG22	3:U:172:LYS:H	1.77	0.48
3:U:194:GLU:HB2	3:U:293:ARG:HD2	1.96	0.48
3:X:200:MET:HE1	3:X:239:LEU:HD21	1.95	0.48
3:X:242:THR:O	3:X:272:ARG:HD3	2.13	0.48
2:R:10:SER:HA	2:R:15:GLU:HB2	1.96	0.48
3:S:242:THR:O	3:S:272:ARG:HD3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:226:ALA:HB3	3:T:268:ARG:HB3	1.95	0.48
3:V:36:LEU:HD21	3:V:297:PHE:HB2	1.96	0.48
3:X:281:LEU:HB3	3:X:284:LEU:HD12	1.96	0.48
1:1:231:ASP:OD2	1:1:321:ARG:NH1	2.47	0.48
3:T:199:PHE:CE1	3:T:242:THR:HG21	2.48	0.48
3:W:11:LEU:HD12	3:W:93:THR:HG21	1.96	0.48
3:X:4:GLN:HB2	3:X:97:GLN:HB3	1.96	0.48
3:T:26:VAL:HG23	3:T:67:THR:HG22	1.96	0.48
3:V:144:PHE:HB3	3:V:190:TRP:CE2	2.49	0.48
1:Z:231:ASP:OD2	1:Z:321:ARG:NH1	2.47	0.48
3:T:212:ALA:HB2	3:T:283:ASN:HD22	1.79	0.47
3:U:106:ASP:O	3:U:133:ILE:HB	2.14	0.47
3:W:171:ILE:HG22	3:W:172:LYS:H	1.79	0.47
2:D:49:THR:HG22	3:S:232:GLU:HB2	1.96	0.47
3:S:242:THR:HG23	3:S:272:ARG:HG3	1.89	0.47
1:1:169:THR:HG21	1:Y:294:PHE:CE2	2.50	0.47
2:P:148:ILE:HB	2:R:153:MET:HG3	1.96	0.47
2:P:172:ASN:HD21	2:P:204:SER:H	1.63	0.47
3:S:281:LEU:HB3	3:S:284:LEU:HD12	1.96	0.47
1:Y:45:GLU:HA	1:Y:357:THR:HG22	1.95	0.47
3:U:4:GLN:HB2	3:U:97:GLN:HB3	1.97	0.47
2:M:172:ASN:HD21	2:M:204:SER:H	1.62	0.46
3:S:194:GLU:HB2	3:S:293:ARG:HD2	1.97	0.46
3:X:196:ILE:HD13	3:X:291:ILE:HG13	1.97	0.46
1:1:42:ILE:HD13	3:X:43:TRP:NE1	2.30	0.46
3:V:160:TYR:HB3	3:V:166:GLY:HA3	1.95	0.46
3:V:196:ILE:HD13	3:V:291:ILE:HG12	1.97	0.46
3:W:72:LEU:HD22	3:W:76:TYR:CE2	2.50	0.46
3:X:72:LEU:HD22	3:X:76:TYR:CE2	2.51	0.46
2:A:77:LYS:H	2:A:82:ASN:ND2	2.11	0.46
2:R:27:TYR:HA	2:R:30:LEU:HD12	1.97	0.46
3:U:72:LEU:HD22	3:U:76:TYR:CE2	2.51	0.46
1:1:212:ASN:ND2	2:N:79:ASP:O	2.46	0.46
2:E:171:GLY:HA3	2:E:205:GLY:H	1.81	0.46
2:M:148:ILE:HB	2:O:153:MET:HG3	1.98	0.46
2:N:171:GLY:HA3	2:N:205:GLY:H	1.81	0.46
3:V:196:ILE:HG22	3:V:293:ARG:HD3	1.98	0.46
1:Y:251:LYS:HG2	1:Y:297:ARG:HD3	1.97	0.46
3:S:72:LEU:HD22	3:S:76:TYR:CE2	2.50	0.46
2:B:171:GLY:HA3	2:B:205:GLY:H	1.81	0.46
2:M:5:ASN:HB3	2:M:8:PHE:CD1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:73:GLU:HG3	3:T:100:ILE:HG23	1.98	0.46
3:T:96:TYR:HB3	3:T:103:VAL:HG23	1.98	0.46
3:U:206:LYS:HG3	3:U:285:SER:HB3	1.98	0.46
3:U:272:ARG:NH1	1:Z:3:GLU:OE1	2.49	0.46
2:D:172:ASN:HD21	2:D:204:SER:H	1.64	0.46
2:P:9:PHE:HA	3:X:160:TYR:HB2	1.97	0.46
3:V:243:ASP:OD1	3:V:245:ASN:N	2.48	0.46
3:T:72:LEU:HD22	3:T:76:TYR:CE2	2.51	0.46
3:V:72:LEU:HD22	3:V:76:TYR:CE2	2.50	0.46
1:Y:122:PRO:HD2	1:Y:125:ILE:HD12	1.96	0.46
1:Z:130:ASN:HA	1:Z:133:ILE:HD12	1.98	0.46
1:1:42:ILE:HD13	3:X:43:TRP:HE1	1.81	0.45
1:1:218:ILE:HG12	2:N:79:ASP:OD2	2.16	0.45
3:T:144:PHE:HB3	3:T:190:TRP:CE2	2.52	0.45
2:Q:251:THR:HA	2:Q:252:PRO:HD3	1.86	0.45
3:V:246:ASP:CG	3:V:246:ASP:O	2.59	0.45
2:J:39:ARG:HB2	2:J:61:ILE:HB	1.99	0.45
2:K:171:GLY:HA3	2:K:205:GLY:H	1.81	0.45
3:T:242:THR:O	3:T:272:ARG:HD3	2.16	0.45
3:X:96:TYR:HB3	3:X:103:VAL:HG23	1.98	0.45
1:Z:230:MET:HE3	1:Z:320:THR:HG21	1.99	0.45
2:B:26:LEU:HD13	2:C:66:TYR:HB2	1.99	0.45
2:G:172:ASN:HD21	2:G:204:SER:H	1.63	0.45
2:J:172:ASN:HD21	2:J:204:SER:H	1.63	0.45
2:M:66:TYR:HB2	2:O:26:LEU:HD13	1.99	0.45
3:T:240:ILE:HG22	3:T:249:TYR:HD1	1.82	0.45
1:Y:130:ASN:HA	1:Y:133:ILE:HD12	1.99	0.45
3:W:144:PHE:HB3	3:W:190:TRP:CE2	2.52	0.45
3:T:266:PHE:HB3	1:Z:221:ARG:HB2	1.99	0.45
3:U:229:PHE:CE1	3:U:264:MET:HB3	2.52	0.45
1:1:130:ASN:HA	1:1:133:ILE:HD12	1.98	0.45
2:H:26:LEU:HD13	2:I:66:TYR:HB2	1.99	0.45
2:P:39:ARG:HB2	2:P:61:ILE:HB	1.99	0.45
2:M:27:TYR:HA	2:M:30:LEU:HD12	1.99	0.45
3:U:69:GLY:H	3:U:75:ASN:HD21	1.64	0.45
1:1:292:THR:HB	1:Z:120:ASP:HB2	1.98	0.44
2:Q:171:GLY:HA3	2:Q:205:GLY:H	1.81	0.44
2:R:5:ASN:HB3	2:R:8:PHE:CD1	2.51	0.44
2:R:81:VAL:HG22	2:R:127:THR:HG23	1.99	0.44
3:S:118:TYR:HB3	3:S:122:GLY:HA2	1.99	0.44
3:U:96:TYR:HB3	3:U:103:VAL:HG23	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:VAL:HG22	2:C:127:THR:HG23	1.99	0.44
2:A:66:TYR:HB2	2:C:26:LEU:HD13	1.99	0.44
2:E:26:LEU:HD13	2:F:66:TYR:HB2	1.98	0.44
2:H:171:GLY:HA3	2:H:205:GLY:H	1.81	0.44
1:Z:251:LYS:HG2	1:Z:297:ARG:HD3	1.98	0.44
3:U:144:PHE:HB3	3:U:190:TRP:CE2	2.52	0.44
1:Z:1:MET:HG3	1:Z:40:GLN:HB2	2.00	0.44
1:1:220:THR:HG21	1:1:332:LEU:HD21	2.00	0.44
2:J:77:LYS:H	2:J:82:ASN:ND2	2.12	0.44
2:J:251:THR:HA	2:J:252:PRO:HD3	1.87	0.44
2:R:9:PHE:HZ	3:X:181:GLU:HG3	1.73	0.44
3:V:194:GLU:HB2	3:V:293:ARG:HD2	1.99	0.44
2:F:39:ARG:HB2	2:F:61:ILE:HB	2.00	0.44
2:L:81:VAL:HG22	2:L:127:THR:HG23	2.00	0.44
2:O:81:VAL:HG22	2:O:127:THR:HG23	1.99	0.44
3:S:138:THR:O	3:S:292:LYS:HA	2.17	0.44
3:T:136:TRP:HB2	3:T:295:ALA:O	2.17	0.44
3:U:229:PHE:CD1	3:U:260:LEU:HB3	2.52	0.44
1:Z:32:LEU:HD11	1:Z:204:LEU:HB2	1.99	0.44
1:1:72:LEU:HD22	3:W:270:ARG:NH1	2.33	0.44
2:G:9:PHE:HA	3:U:160:TYR:HB2	2.00	0.44
2:K:26:LEU:HD13	2:L:66:TYR:HB2	2.00	0.44
2:K:251:THR:HA	2:K:252:PRO:HD3	1.90	0.44
3:S:11:LEU:HD12	3:S:93:THR:HG21	1.99	0.44
3:W:194:GLU:HB2	3:W:293:ARG:HD2	1.99	0.44
2:A:172:ASN:ND2	2:A:204:SER:H	2.16	0.44
2:C:39:ARG:HB2	2:C:61:ILE:HB	2.00	0.44
3:S:96:TYR:HB3	3:S:103:VAL:HG23	1.99	0.44
1:Y:1:MET:HG3	1:Y:40:GLN:HB2	1.99	0.44
1:Y:41:VAL:HG11	1:Y:71:ILE:HG12	2.00	0.44
2:G:77:LYS:H	2:G:82:ASN:ND2	2.12	0.44
3:S:239:LEU:HD23	3:S:240:ILE:N	2.32	0.44
3:W:3:ARG:HD2	3:W:3:ARG:C	2.42	0.44
3:W:247:GLU:OE1	3:W:249:TYR:HE2	2.01	0.44
3:X:198:SER:HA	3:X:242:THR:OG1	2.18	0.44
2:D:39:ARG:HB2	2:D:61:ILE:HB	2.00	0.43
2:D:146:ASP:O	2:F:151:ASN:HB2	2.17	0.43
2:E:17:PRO:CB	3:T:167:ASN:HB2	2.48	0.43
2:F:81:VAL:HG22	2:F:127:THR:HG23	1.99	0.43
2:O:27:TYR:HA	2:O:30:LEU:HD12	2.00	0.43
1:1:152:PHE:C	1:1:152:PHE:CD2	2.96	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:THR:HG21	3:S:258:LEU:HD21	2.00	0.43
2:J:148:ILE:HB	2:L:153:MET:HG3	1.99	0.43
3:T:40:ASN:HB3	3:T:51:MET:HE3	1.99	0.43
3:X:5:TYR:HB3	3:X:21:VAL:HG23	2.00	0.43
3:X:243:ASP:OD1	3:X:243:ASP:C	2.60	0.43
2:I:81:VAL:HG22	2:I:127:THR:HG23	1.99	0.43
2:M:39:ARG:HB2	2:M:61:ILE:HB	2.00	0.43
2:R:39:ARG:HB2	2:R:61:ILE:HB	2.00	0.43
3:S:40:ASN:HB3	3:S:51:MET:HE3	2.00	0.43
3:S:132:ILE:HG21	3:S:135:LYS:HB2	2.00	0.43
3:U:203:LEU:HB2	3:U:238:ILE:HB	2.01	0.43
3:V:40:ASN:HB3	3:V:51:MET:HE3	2.00	0.43
1:Z:184:GLN:HE22	1:Z:217:ARG:HH22	1.66	0.43
2:O:155:VAL:HG21	2:O:159:ILE:HD11	2.01	0.43
3:T:202:ILE:HG12	3:T:239:LEU:HD12	2.01	0.43
1:1:39:CYS:HB2	1:1:60:THR:OG1	2.18	0.43
2:A:39:ARG:HB2	2:A:61:ILE:HB	2.00	0.43
3:X:196:ILE:HD11	3:X:199:PHE:HD1	1.84	0.43
2:P:77:LYS:H	2:P:82:ASN:ND2	2.12	0.43
3:U:242:THR:CG2	3:U:272:ARG:CG	2.93	0.43
3:W:196:ILE:HD11	3:W:199:PHE:HD1	1.83	0.43
2:E:155:VAL:HG21	2:E:159:ILE:HD11	2.00	0.43
2:G:203:MET:SD	2:G:243:TRP:HB2	2.59	0.43
2:O:39:ARG:HB2	2:O:61:ILE:HB	2.00	0.43
3:W:40:ASN:HB3	3:W:51:MET:HE3	2.00	0.43
2:G:39:ARG:HB2	2:G:61:ILE:HB	2.00	0.43
2:I:39:ARG:HB2	2:I:61:ILE:HB	2.00	0.43
2:O:5:ASN:HB3	2:O:8:PHE:CD1	2.54	0.43
2:Q:155:VAL:HG21	2:Q:159:ILE:HD11	2.01	0.43
3:T:137:TYR:CE1	3:T:292:LYS:HD2	2.54	0.43
3:U:270:ARG:NH2	1:Z:90:ASN:HB3	2.33	0.43
1:1:1:MET:HG3	1:1:40:GLN:HB2	2.00	0.43
2:B:19:GLY:HA2	3:S:166:GLY:O	2.19	0.43
2:N:26:LEU:HD13	2:O:66:TYR:HB2	2.01	0.43
3:X:243:ASP:OD1	3:X:245:ASN:N	2.52	0.42
1:Y:152:PHE:C	1:Y:152:PHE:CD2	2.96	0.42
2:G:172:ASN:ND2	2:G:204:SER:H	2.17	0.42
2:H:155:VAL:HG21	2:H:159:ILE:HD11	2.01	0.42
2:N:51:LEU:HD12	3:V:262:PRO:HG2	2.02	0.42
3:T:86:ILE:HA	3:T:92:VAL:HG21	2.01	0.42
3:U:40:ASN:HB3	3:U:51:MET:HE3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:52:LEU:HD23	1:Y:53:TYR:CE2	2.55	0.42
3:W:247:GLU:OE1	3:W:249:TYR:CE2	2.73	0.42
2:G:174:LEU:HB2	2:G:194:VAL:HG22	2.02	0.42
3:W:199:PHE:CE1	3:W:242:THR:HG21	2.55	0.42
2:D:203:MET:SD	2:D:243:TRP:HB2	2.60	0.42
2:F:155:VAL:HG21	2:F:159:ILE:HD11	2.01	0.42
2:B:251:THR:HA	2:B:252:PRO:HD3	1.93	0.42
2:H:251:THR:HA	2:H:252:PRO:HD3	1.89	0.42
2:I:5:ASN:HB3	2:I:8:PHE:CD1	2.55	0.42
3:U:226:ALA:HB3	3:U:268:ARG:HB3	2.01	0.42
1:I:12:PRO:HB2	1:Y:288:ARG:CZ	2.49	0.42
2:C:155:VAL:HG21	2:C:159:ILE:HD11	2.02	0.42
2:M:77:LYS:H	2:M:82:ASN:ND2	2.13	0.42
3:W:96:TYR:HB3	3:W:103:VAL:HG23	2.02	0.42
3:W:196:ILE:HD13	3:W:291:ILE:HG12	2.02	0.42
2:D:77:LYS:H	2:D:82:ASN:ND2	2.12	0.42
3:X:3:ARG:HD2	3:X:3:ARG:C	2.45	0.42
1:I:323:ILE:HA	1:I:363:LEU:O	2.20	0.42
3:T:171:ILE:H	3:T:175:SER:HA	1.84	0.42
1:Y:121:VAL:HG11	1:Y:175:VAL:HG21	2.01	0.42
1:Z:77:VAL:O	1:Z:89:LEU:HB3	2.20	0.41
2:L:39:ARG:HB2	2:L:61:ILE:HB	2.00	0.41
2:M:5:ASN:O	2:M:16:PHE:HB3	2.20	0.41
3:S:54:ARG:NH1	3:X:87:LEU:HA	2.35	0.41
3:W:281:LEU:HB3	3:W:284:LEU:HD12	2.03	0.41
2:F:27:TYR:HA	2:F:30:LEU:HD12	2.01	0.41
1:Y:323:ILE:HA	1:Y:363:LEU:O	2.20	0.41
2:G:66:TYR:HB2	2:I:26:LEU:HD13	2.02	0.41
2:J:203:MET:SD	2:J:243:TRP:HB2	2.60	0.41
2:R:155:VAL:HG21	2:R:159:ILE:HD11	2.02	0.41
3:S:7:ILE:HG23	3:S:92:VAL:CG1	2.51	0.41
3:S:171:ILE:H	3:S:175:SER:HA	1.85	0.41
3:V:87:LEU:HA	3:W:54:ARG:NH1	2.36	0.41
2:A:198:GLN:HB2	2:A:201:TRP:CD1	2.56	0.41
2:D:174:LEU:HB2	2:D:194:VAL:HG22	2.02	0.41
2:L:10:SER:HA	2:L:15:GLU:HB2	2.03	0.41
3:V:118:TYR:HB3	3:V:122:GLY:HA2	2.02	0.41
1:I:52:LEU:HD23	1:I:53:TYR:CE2	2.56	0.41
3:U:203:LEU:HD13	3:U:213:GLY:HA2	2.01	0.41
3:V:199:PHE:CZ	3:V:242:THR:HG21	2.55	0.41
1:Z:241:TYR:CD2	1:Z:241:TYR:N	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5:ASN:HB3	2:G:8:PHE:CD1	2.56	0.41
2:L:5:ASN:HB3	2:L:8:PHE:CD1	2.56	0.41
2:M:174:LEU:HB2	2:M:194:VAL:HG22	2.03	0.41
2:P:5:ASN:HD21	2:Q:97:VAL:HB	1.85	0.41
3:U:171:ILE:H	3:U:175:SER:HA	1.86	0.41
1:1:76:VAL:HG21	1:1:88:LYS:HE3	2.02	0.41
1:1:152:PHE:C	1:1:152:PHE:HD2	2.29	0.41
1:1:294:PHE:CE2	1:Z:169:THR:CG2	3.03	0.41
2:D:147:SER:HB2	2:E:140:VAL:HG22	2.02	0.41
2:E:27:TYR:HA	2:E:30:LEU:HD12	2.03	0.41
2:N:155:VAL:HG21	2:N:159:ILE:HD11	2.01	0.41
2:P:146:ASP:O	2:R:151:ASN:HB2	2.21	0.41
3:T:158:LYS:HD2	3:T:176:TYR:CE1	2.56	0.41
1:Z:348:SER:O	1:Z:367:GLU:HG3	2.21	0.41
2:D:172:ASN:ND2	2:D:204:SER:H	2.19	0.41
2:J:174:LEU:HB2	2:J:194:VAL:HG22	2.04	0.40
2:P:172:ASN:ND2	2:P:204:SER:H	2.19	0.40
3:T:11:LEU:O	3:T:12:ASP:CG	2.64	0.40
3:T:199:PHE:HB3	3:T:291:ILE:HD13	2.02	0.40
3:W:171:ILE:H	3:W:175:SER:HA	1.86	0.40
1:Y:175:VAL:HG12	1:Y:178:ARG:HH12	1.86	0.40
2:E:229:THR:HB	2:F:228:ASP:HB2	2.03	0.40
2:J:172:ASN:ND2	2:J:204:SER:H	2.19	0.40
2:K:229:THR:HB	2:L:228:ASP:HB2	2.03	0.40
2:M:172:ASN:ND2	2:M:204:SER:H	2.19	0.40
2:B:229:THR:HB	2:C:228:ASP:HB2	2.03	0.40
3:V:240:ILE:CD1	3:V:242:THR:HG23	2.51	0.40
2:A:229:THR:HB	2:B:228:ASP:HB2	2.04	0.40
3:T:114:LYS:HB3	3:U:34:LEU:HB2	2.04	0.40
1:Z:52:LEU:HD23	1:Z:53:TYR:CE2	2.56	0.40
2:A:251:THR:HA	2:A:252:PRO:HD3	1.95	0.40
2:Q:229:THR:HB	2:R:228:ASP:HB2	2.03	0.40
3:S:3:ARG:C	3:S:3:ARG:HD2	2.46	0.40
3:S:239:LEU:C	3:S:239:LEU:CD2	2.94	0.40
1:Y:185:PHE:CE2	1:Y:208:PHE:HA	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	370/375 (99%)	358 (97%)	12 (3%)	0	100	100
1	Y	370/375 (99%)	355 (96%)	15 (4%)	0	100	100
1	Z	370/375 (99%)	357 (96%)	13 (4%)	0	100	100
2	A	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	B	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	C	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	D	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	E	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	F	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	G	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	H	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	I	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	J	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	K	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	L	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	M	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
2	N	261/263 (99%)	247 (95%)	14 (5%)	0	100	100
2	O	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
2	P	261/263 (99%)	254 (97%)	7 (3%)	0	100	100
2	Q	261/263 (99%)	245 (94%)	16 (6%)	0	100	100
2	R	261/263 (99%)	246 (94%)	15 (6%)	0	100	100
3	S	296/298 (99%)	278 (94%)	16 (5%)	2 (1%)	18	53
3	T	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	18	53
3	U	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	18	53
3	V	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	18	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	W	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	18	53
3	X	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	18	53
All	All	7584/7647 (99%)	7207 (95%)	365 (5%)	12 (0%)	43	74

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	175	SER
3	T	175	SER
3	U	175	SER
3	V	175	SER
3	W	175	SER
3	X	175	SER
3	S	136	TRP
3	U	136	TRP
3	V	136	TRP
3	W	136	TRP
3	X	136	TRP
3	T	136	TRP

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	337/340 (99%)	323 (96%)	14 (4%)	26	50
1	Y	337/340 (99%)	319 (95%)	18 (5%)	20	46
1	Z	337/340 (99%)	318 (94%)	19 (6%)	19	45
2	A	227/227 (100%)	217 (96%)	10 (4%)	25	49
2	B	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	C	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	D	227/227 (100%)	219 (96%)	8 (4%)	32	54
2	E	227/227 (100%)	223 (98%)	4 (2%)	51	67

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	G	227/227 (100%)	218 (96%)	9 (4%)	28	51
2	H	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	I	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	J	227/227 (100%)	218 (96%)	9 (4%)	28	51
2	K	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	L	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	M	227/227 (100%)	218 (96%)	9 (4%)	28	51
2	N	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	O	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	P	227/227 (100%)	218 (96%)	9 (4%)	28	51
2	Q	227/227 (100%)	223 (98%)	4 (2%)	51	67
2	R	227/227 (100%)	222 (98%)	5 (2%)	45	64
3	S	264/264 (100%)	240 (91%)	24 (9%)	9	31
3	T	264/264 (100%)	242 (92%)	22 (8%)	10	34
3	U	264/264 (100%)	235 (89%)	29 (11%)	6	24
3	V	264/264 (100%)	235 (89%)	29 (11%)	6	24
3	W	264/264 (100%)	231 (88%)	33 (12%)	4	20
3	X	264/264 (100%)	239 (90%)	25 (10%)	8	29
All	All	6681/6690 (100%)	6365 (95%)	316 (5%)	23	48

All (316) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	LEU
1	1	8	ASP
1	1	40	GLN
1	1	42	ILE
1	1	88	LYS
1	1	96	LEU
1	1	152	PHE
1	1	224	ILE
1	1	238	ARG
1	1	286	ASP
1	1	313	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	319	VAL
1	1	330	LEU
1	1	360	ASN
2	A	2	THR
2	A	7	THR
2	A	9	PHE
2	A	18	VAL
2	A	38	ILE
2	A	79	ASP
2	A	93	THR
2	A	124	ASP
2	A	202	ASN
2	A	233	ILE
2	B	38	ILE
2	B	84	ILE
2	B	206	THR
2	B	232	HIS
2	C	7	THR
2	C	38	ILE
2	C	125	ILE
2	C	232	HIS
2	D	9	PHE
2	D	18	VAL
2	D	38	ILE
2	D	79	ASP
2	D	93	THR
2	D	124	ASP
2	D	202	ASN
2	D	233	ILE
2	E	38	ILE
2	E	84	ILE
2	E	206	THR
2	E	232	HIS
2	F	7	THR
2	F	38	ILE
2	F	125	ILE
2	F	232	HIS
2	G	7	THR
2	G	9	PHE
2	G	18	VAL
2	G	38	ILE
2	G	79	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	93	THR
2	G	124	ASP
2	G	202	ASN
2	G	233	ILE
2	H	38	ILE
2	H	84	ILE
2	H	206	THR
2	H	232	HIS
2	I	7	THR
2	I	38	ILE
2	I	125	ILE
2	I	232	HIS
2	J	7	THR
2	J	9	PHE
2	J	18	VAL
2	J	38	ILE
2	J	79	ASP
2	J	93	THR
2	J	124	ASP
2	J	202	ASN
2	J	233	ILE
2	K	38	ILE
2	K	84	ILE
2	K	206	THR
2	K	232	HIS
2	L	26	LEU
2	L	38	ILE
2	L	125	ILE
2	L	232	HIS
2	M	7	THR
2	M	9	PHE
2	M	18	VAL
2	M	38	ILE
2	M	79	ASP
2	M	93	THR
2	M	124	ASP
2	M	202	ASN
2	M	233	ILE
2	N	38	ILE
2	N	84	ILE
2	N	206	THR
2	N	232	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	7	THR
2	O	38	ILE
2	O	125	ILE
2	O	232	HIS
2	P	7	THR
2	P	9	PHE
2	P	18	VAL
2	P	38	ILE
2	P	79	ASP
2	P	93	THR
2	P	124	ASP
2	P	202	ASN
2	P	233	ILE
2	Q	38	ILE
2	Q	84	ILE
2	Q	206	THR
2	Q	232	HIS
2	R	7	THR
2	R	26	LEU
2	R	38	ILE
2	R	125	ILE
2	R	232	HIS
3	S	2	VAL
3	S	11	LEU
3	S	26	VAL
3	S	43	TRP
3	S	48	ILE
3	S	54	ARG
3	S	55	SER
3	S	64	LYS
3	S	66	GLU
3	S	72	LEU
3	S	109	LEU
3	S	123	THR
3	S	142	LEU
3	S	159	ILE
3	S	171	ILE
3	S	196	ILE
3	S	227	ILE
3	S	228	VAL
3	S	234	VAL
3	S	256	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	S	263	VAL
3	S	270	ARG
3	S	291	ILE
3	S	294	LYS
3	T	2	VAL
3	T	11	LEU
3	T	26	VAL
3	T	36	LEU
3	T	48	ILE
3	T	55	SER
3	T	64	LYS
3	T	65	LEU
3	T	72	LEU
3	T	123	THR
3	T	135	LYS
3	T	159	ILE
3	T	169	LYS
3	T	171	ILE
3	T	196	ILE
3	T	203	LEU
3	T	234	VAL
3	T	236	ASP
3	T	239	LEU
3	T	243	ASP
3	T	263	VAL
3	T	294	LYS
3	U	2	VAL
3	U	3	ARG
3	U	11	LEU
3	U	26	VAL
3	U	37	GLN
3	U	39	THR
3	U	43	TRP
3	U	48	ILE
3	U	53	THR
3	U	54	ARG
3	U	55	SER
3	U	64	LYS
3	U	66	GLU
3	U	72	LEU
3	U	135	LYS
3	U	142	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	U	159	ILE
3	U	171	ILE
3	U	196	ILE
3	U	228	VAL
3	U	232	GLU
3	U	234	VAL
3	U	244	VAL
3	U	256	THR
3	U	258	LEU
3	U	263	VAL
3	U	282	ILE
3	U	291	ILE
3	U	294	LYS
3	V	2	VAL
3	V	11	LEU
3	V	36	LEU
3	V	48	ILE
3	V	54	ARG
3	V	55	SER
3	V	64	LYS
3	V	66	GLU
3	V	72	LEU
3	V	120	LYS
3	V	135	LYS
3	V	142	LEU
3	V	143	THR
3	V	159	ILE
3	V	169	LYS
3	V	196	ILE
3	V	203	LEU
3	V	227	ILE
3	V	232	GLU
3	V	234	VAL
3	V	240	ILE
3	V	243	ASP
3	V	246	ASP
3	V	256	THR
3	V	258	LEU
3	V	263	VAL
3	V	282	ILE
3	V	291	ILE
3	V	294	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	W	2	VAL
3	W	6	LYS
3	W	11	LEU
3	W	26	VAL
3	W	43	TRP
3	W	48	ILE
3	W	54	ARG
3	W	55	SER
3	W	64	LYS
3	W	66	GLU
3	W	72	LEU
3	W	92	VAL
3	W	109	LEU
3	W	123	THR
3	W	143	THR
3	W	159	ILE
3	W	169	LYS
3	W	171	ILE
3	W	196	ILE
3	W	197	PHE
3	W	203	LEU
3	W	228	VAL
3	W	232	GLU
3	W	234	VAL
3	W	244	VAL
3	W	248	THR
3	W	256	THR
3	W	258	LEU
3	W	263	VAL
3	W	270	ARG
3	W	282	ILE
3	W	291	ILE
3	W	294	LYS
3	X	2	VAL
3	X	11	LEU
3	X	26	VAL
3	X	36	LEU
3	X	43	TRP
3	X	48	ILE
3	X	54	ARG
3	X	64	LYS
3	X	66	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	X	72	LEU
3	X	107	LEU
3	X	142	LEU
3	X	159	ILE
3	X	169	LYS
3	X	171	ILE
3	X	196	ILE
3	X	200	MET
3	X	203	LEU
3	X	228	VAL
3	X	234	VAL
3	X	243	ASP
3	X	244	VAL
3	X	258	LEU
3	X	263	VAL
3	X	291	ILE
1	Y	8	ASP
1	Y	26	LYS
1	Y	40	GLN
1	Y	41	VAL
1	Y	87	LYS
1	Y	88	LYS
1	Y	96	LEU
1	Y	152	PHE
1	Y	192	GLN
1	Y	242	ASN
1	Y	243	PHE
1	Y	286	ASP
1	Y	306	LEU
1	Y	313	ILE
1	Y	319	VAL
1	Y	330	LEU
1	Y	340	ILE
1	Y	360	ASN
1	Z	2	LEU
1	Z	8	ASP
1	Z	26	LYS
1	Z	39	CYS
1	Z	40	GLN
1	Z	41	VAL
1	Z	88	LYS
1	Z	96	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Z	151	PHE
1	Z	165	ARG
1	Z	207	ASN
1	Z	218	ILE
1	Z	238	ARG
1	Z	286	ASP
1	Z	313	ILE
1	Z	319	VAL
1	Z	320	THR
1	Z	340	ILE
1	Z	360	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (152) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	11	ASN
1	1	43	ASN
1	1	143	ASN
1	1	184	GLN
1	1	214	ASN
1	1	267	ASN
2	A	48	ASN
2	A	71	ASN
2	A	82	ASN
2	A	92	GLN
2	A	172	ASN
2	A	236	ASN
2	B	48	ASN
2	B	57	ASN
2	B	164	GLN
2	C	57	ASN
2	C	172	ASN
2	C	236	ASN
2	D	48	ASN
2	D	57	ASN
2	D	71	ASN
2	D	82	ASN
2	D	92	GLN
2	D	172	ASN
2	D	196	ASN
2	D	236	ASN
2	E	48	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	57	ASN
2	E	164	GLN
2	F	54	GLN
2	F	57	ASN
2	F	71	ASN
2	F	172	ASN
2	F	236	ASN
2	G	48	ASN
2	G	57	ASN
2	G	71	ASN
2	G	82	ASN
2	G	92	GLN
2	G	172	ASN
2	G	196	ASN
2	G	236	ASN
2	H	48	ASN
2	H	57	ASN
2	H	164	GLN
2	H	177	GLN
2	H	218	GLN
2	I	54	GLN
2	I	57	ASN
2	I	71	ASN
2	I	172	ASN
2	I	236	ASN
2	I	258	ASN
2	J	48	ASN
2	J	57	ASN
2	J	71	ASN
2	J	82	ASN
2	J	172	ASN
2	J	196	ASN
2	J	236	ASN
2	K	48	ASN
2	K	57	ASN
2	K	164	GLN
2	K	177	GLN
2	L	57	ASN
2	L	172	ASN
2	L	236	ASN
2	M	48	ASN
2	M	57	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	71	ASN
2	M	82	ASN
2	M	172	ASN
2	M	196	ASN
2	M	236	ASN
2	N	48	ASN
2	N	57	ASN
2	N	92	GLN
2	N	164	GLN
2	N	218	GLN
2	O	57	ASN
2	O	172	ASN
2	O	236	ASN
2	O	258	ASN
2	P	5	ASN
2	P	48	ASN
2	P	57	ASN
2	P	71	ASN
2	P	82	ASN
2	P	172	ASN
2	P	196	ASN
2	P	236	ASN
2	Q	57	ASN
2	Q	164	GLN
2	Q	177	GLN
2	R	48	ASN
2	R	54	GLN
2	R	57	ASN
2	R	71	ASN
2	R	172	ASN
2	R	236	ASN
3	S	77	GLN
3	S	102	GLN
3	S	250	GLN
3	S	259	ASN
3	T	4	GLN
3	T	23	ASN
3	T	141	ASN
3	T	167	ASN
3	T	235	GLN
3	T	259	ASN
3	U	23	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	U	37	GLN
3	U	75	ASN
3	U	77	GLN
3	U	97	GLN
3	U	141	ASN
3	U	250	GLN
3	U	259	ASN
3	V	23	ASN
3	V	97	GLN
3	V	141	ASN
3	V	235	GLN
3	V	250	GLN
3	V	259	ASN
3	W	235	GLN
3	W	245	ASN
3	X	44	GLN
3	X	77	GLN
3	X	141	ASN
3	X	167	ASN
3	X	235	GLN
3	X	250	GLN
3	X	259	ASN
1	Y	11	ASN
1	Y	24	ASN
1	Y	40	GLN
1	Y	90	ASN
1	Y	123	ASN
1	Y	164	ASN
1	Y	186	GLN
1	Y	212	ASN
1	Y	214	ASN
1	Y	267	ASN
1	Z	11	ASN
1	Z	16	ASN
1	Z	24	ASN
1	Z	130	ASN
1	Z	164	ASN
1	Z	184	GLN
1	Z	192	GLN
1	Z	214	ASN
1	Z	267	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	372/375 (99%)	0.75	18 (4%) 35 27	63, 97, 170, 239	0
1	Y	372/375 (99%)	0.60	11 (2%) 52 36	62, 94, 151, 270	0
1	Z	372/375 (99%)	0.66	19 (5%) 33 26	63, 98, 166, 246	0
2	A	263/263 (100%)	0.49	6 (2%) 61 43	44, 76, 105, 140	0
2	B	263/263 (100%)	0.44	9 (3%) 48 34	55, 88, 126, 147	0
2	C	263/263 (100%)	0.54	4 (1%) 72 50	55, 90, 137, 172	0
2	D	263/263 (100%)	0.76	13 (4%) 35 27	52, 106, 248, 290	0
2	E	263/263 (100%)	0.99	34 (12%) 7 10	64, 121, 259, 286	0
2	F	263/263 (100%)	1.11	30 (11%) 10 13	57, 144, 245, 291	0
2	G	263/263 (100%)	0.89	20 (7%) 20 19	60, 126, 249, 285	0
2	H	263/263 (100%)	1.19	45 (17%) 4 7	97, 155, 233, 282	0
2	I	263/263 (100%)	1.12	42 (15%) 5 8	75, 156, 262, 297	0
2	J	263/263 (100%)	0.60	12 (4%) 37 28	55, 102, 163, 246	0
2	K	263/263 (100%)	0.61	6 (2%) 61 43	52, 84, 175, 233	0
2	L	263/263 (100%)	0.76	18 (6%) 23 21	62, 102, 162, 220	0
2	M	263/263 (100%)	0.80	17 (6%) 25 22	76, 126, 166, 208	0
2	N	263/263 (100%)	0.77	16 (6%) 27 23	60, 95, 142, 163	0
2	O	263/263 (100%)	0.88	18 (6%) 23 21	85, 128, 168, 184	0
2	P	263/263 (100%)	0.99	24 (9%) 15 16	65, 132, 296, 298	0
2	Q	263/263 (100%)	1.25	40 (15%) 5 8	96, 154, 288, 292	0
2	R	263/263 (100%)	1.10	38 (14%) 6 9	83, 160, 292, 300	0
3	S	298/298 (100%)	0.58	7 (2%) 61 43	41, 64, 106, 124	0
3	T	298/298 (100%)	0.48	9 (3%) 52 36	42, 65, 113, 145	0
3	U	298/298 (100%)	0.55	12 (4%) 42 31	43, 71, 129, 169	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	V	298/298 (100%)	0.47	8 (2%) 56 39	44, 66, 101, 127	0
3	W	298/298 (100%)	0.58	12 (4%) 42 31	40, 67, 132, 161	0
3	X	298/298 (100%)	0.61	16 (5%) 31 25	40, 67, 158, 202	0
All	All	7638/7647 (99%)	0.75	504 (6%) 24 21	40, 98, 207, 300	0

All (504) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Q	222	GLY	7.7
2	Q	221	VAL	6.7
2	E	221	VAL	6.1
2	F	221	VAL	6.0
2	H	184	ASP	6.0
2	P	221	VAL	5.9
2	F	222	GLY	5.5
2	F	260	SER	5.1
2	P	222	GLY	5.0
2	F	259	GLY	4.8
2	P	64	GLY	4.8
2	F	257	GLY	4.7
2	H	221	VAL	4.7
2	L	228	ASP	4.6
2	L	184	ASP	4.6
2	D	221	VAL	4.5
2	Q	228	ASP	4.5
2	P	231	PHE	4.5
2	H	176	LEU	4.3
2	P	167	THR	4.3
3	S	117	GLY	4.3
2	Q	4	LYS	4.2
2	R	190	PHE	4.2
2	R	221	VAL	4.2
2	E	179	THR	4.1
2	G	64	GLY	4.1
2	L	222	GLY	4.1
2	R	257	GLY	4.1
2	I	241	ILE	4.1
2	O	222	GLY	4.0
2	Q	220	LEU	3.9
2	I	233	ILE	3.8
2	O	27	TYR	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	X	170	TYR	3.8
2	Q	3	ILE	3.7
2	R	253	ILE	3.7
2	K	221	VAL	3.7
1	Z	163	ILE	3.7
2	E	228	ASP	3.7
2	B	246	ALA	3.7
2	E	225	ALA	3.7
2	H	62	ALA	3.7
2	H	220	LEU	3.6
2	I	140	VAL	3.6
2	F	146	ASP	3.6
2	H	235	ILE	3.6
2	O	144	THR	3.5
2	B	23	ASP	3.5
3	W	1	GLY	3.5
2	G	221	VAL	3.5
3	S	174	THR	3.5
1	Z	158	ALA	3.4
2	H	250	LYS	3.4
2	P	176	LEU	3.4
3	U	50	VAL	3.4
1	Z	311	VAL	3.4
2	E	222	GLY	3.4
1	1	163	ILE	3.4
2	H	174	LEU	3.4
2	D	254	ALA	3.4
2	F	225	ALA	3.4
3	X	164	ALA	3.4
2	H	185	LEU	3.3
2	F	241	ILE	3.3
2	R	188	VAL	3.3
2	R	225	ALA	3.3
2	F	188	VAL	3.3
2	I	221	VAL	3.3
2	O	5	ASN	3.3
2	G	17	PRO	3.2
2	B	228	ASP	3.2
2	F	190	PHE	3.2
2	Q	225	ALA	3.2
3	T	99	GLU	3.2
1	1	314	SER	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	161	VAL	3.2
2	M	93	THR	3.2
2	P	145	LEU	3.2
2	E	64	GLY	3.2
2	I	260	SER	3.2
3	V	1	GLY	3.1
3	X	1	GLY	3.1
2	L	144	THR	3.1
3	X	39	THR	3.1
3	X	41	ASN	3.1
1	Y	163	ILE	3.1
2	R	9	PHE	3.1
2	R	255	THR	3.1
2	Q	149	SER	3.1
3	X	159	ILE	3.1
2	H	262	PHE	3.1
2	G	184	ASP	3.1
2	R	241	ILE	3.0
1	Z	33	PRO	3.0
2	H	241	ILE	3.0
2	O	130	GLY	3.0
2	F	185	LEU	3.0
3	X	174	THR	3.0
2	N	199	LYS	2.9
2	D	225	ALA	2.9
2	J	228	ASP	2.9
2	I	201	TRP	2.9
2	E	257	GLY	2.9
2	H	208	VAL	2.9
1	1	122	PRO	2.9
3	X	165	PRO	2.9
2	H	144	THR	2.9
3	V	99	GLU	2.9
2	J	29	MET	2.9
2	I	194	VAL	2.8
2	P	259	GLY	2.8
2	O	220	LEU	2.8
3	W	68	PHE	2.8
2	E	256	ARG	2.8
2	Q	257	GLY	2.8
2	I	75	ALA	2.8
2	I	254	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	144	THR	2.8
2	F	262	PHE	2.8
2	M	90	LEU	2.8
2	I	228	ASP	2.8
2	I	176	LEU	2.8
2	H	261	TYR	2.8
1	Z	192	GLN	2.8
2	D	141	GLN	2.8
2	I	244	TRP	2.8
2	N	149	SER	2.8
2	K	222	GLY	2.8
3	X	43	TRP	2.8
1	Z	303	PRO	2.8
2	R	149	SER	2.8
2	P	144	THR	2.8
2	H	133	VAL	2.7
2	O	8	PHE	2.7
2	Q	9	PHE	2.7
2	R	247	ASN	2.7
2	L	253	ILE	2.7
2	M	184	ASP	2.7
2	Q	130	GLY	2.7
3	X	168	TYR	2.7
2	Q	142	THR	2.7
2	R	176	LEU	2.7
2	I	124	ASP	2.7
2	I	181	LYS	2.7
2	P	233	ILE	2.7
3	X	163	THR	2.7
2	J	221	VAL	2.7
2	O	110	VAL	2.7
2	E	176	LEU	2.7
2	Q	70	LEU	2.7
2	I	215	ALA	2.7
1	1	243	PHE	2.7
2	M	262	PHE	2.7
2	G	18	VAL	2.6
3	W	39	THR	2.6
2	R	29	MET	2.6
2	G	262	PHE	2.6
2	M	231	PHE	2.6
2	I	168	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	241	ILE	2.6
2	G	222	GLY	2.6
1	Z	359	PHE	2.6
2	P	149	SER	2.6
2	M	232	HIS	2.6
2	N	200	GLY	2.6
3	X	155	GLY	2.6
3	W	176	TYR	2.6
2	E	152	ASP	2.6
2	N	79	ASP	2.6
1	Z	318	ILE	2.6
2	N	187	ILE	2.6
2	P	256	ARG	2.6
2	I	232	HIS	2.6
2	P	220	LEU	2.6
2	Q	259	GLY	2.6
2	H	27	TYR	2.6
2	O	23	ASP	2.6
2	Q	227	ARG	2.6
2	I	220	LEU	2.6
2	P	62	ALA	2.6
2	I	222	GLY	2.6
2	L	262	PHE	2.6
2	A	184	ASP	2.6
2	A	196	ASN	2.6
2	E	164	GLN	2.6
2	O	226	GLY	2.6
2	G	223	HIS	2.5
2	F	244	TRP	2.5
2	N	158	SER	2.5
2	R	18	VAL	2.5
1	Z	207	ASN	2.5
2	C	52	ASN	2.5
2	C	160	ASP	2.5
2	Q	21	ASN	2.5
2	H	252	PRO	2.5
2	L	246	ALA	2.5
2	J	226	GLY	2.5
2	B	2	THR	2.5
2	E	144	THR	2.5
2	G	261	TYR	2.5
2	Q	261	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	147	SER	2.5
2	B	18	VAL	2.5
2	A	202	ASN	2.5
1	1	205	PHE	2.5
2	I	190	PHE	2.5
2	F	11	PRO	2.5
2	K	50	ALA	2.5
3	W	154	ALA	2.5
2	L	200	GLY	2.5
3	U	117	GLY	2.5
3	W	159	ILE	2.5
1	Y	348	SER	2.5
2	G	230	SER	2.5
2	H	163	VAL	2.5
3	T	298	VAL	2.5
2	P	33	MET	2.5
1	Z	240	ALA	2.5
3	U	170	TYR	2.5
2	L	95	ASN	2.5
2	O	6	PHE	2.5
2	M	88	ILE	2.5
1	Z	308	THR	2.5
3	S	231	THR	2.5
2	D	261	TYR	2.5
2	I	187	ILE	2.5
2	J	254	ALA	2.5
2	H	222	GLY	2.5
2	I	185	LEU	2.5
2	H	206	THR	2.5
2	H	251	THR	2.5
3	W	174	THR	2.5
2	N	264	LYS	2.4
2	A	201	TRP	2.4
3	U	159	ILE	2.4
2	E	185	LEU	2.4
2	L	23	ASP	2.4
2	R	228	ASP	2.4
2	E	165	THR	2.4
3	U	39	THR	2.4
2	R	140	VAL	2.4
2	M	35	TYR	2.4
2	I	243	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	226	GLY	2.4
1	1	316	SER	2.4
2	F	124	ASP	2.4
2	R	93	THR	2.4
2	P	18	VAL	2.4
2	G	224	PHE	2.4
2	E	27	TYR	2.4
2	G	229	THR	2.4
3	S	115	THR	2.4
1	Z	324	PHE	2.4
1	1	256	TYR	2.4
2	H	178	LEU	2.4
3	V	179	TYR	2.4
2	F	254	ALA	2.4
1	Z	88	LYS	2.4
2	H	13	SER	2.4
2	I	262	PHE	2.4
2	R	136	THR	2.4
3	T	30	GLN	2.4
2	L	243	TRP	2.4
2	O	63	GLY	2.4
3	U	155	GLY	2.4
2	I	251	THR	2.4
2	J	229	THR	2.4
2	L	251	THR	2.4
2	R	47	LEU	2.4
2	R	233	ILE	2.4
2	D	227	ARG	2.4
2	O	228	ASP	2.4
2	H	254	ALA	2.4
2	I	225	ALA	2.4
2	Q	264	LYS	2.4
2	G	182	ASN	2.3
1	1	318	ILE	2.3
2	D	207	TRP	2.3
2	F	220	LEU	2.3
3	V	159	ILE	2.3
3	W	43	TRP	2.3
2	I	136	THR	2.3
2	N	18	VAL	2.3
2	I	234	ASP	2.3
1	Y	324	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	O	16	PHE	2.3
3	T	159	ILE	2.3
3	X	188	SER	2.3
2	E	95	ASN	2.3
2	G	63	GLY	2.3
2	H	57	ASN	2.3
2	M	221	VAL	2.3
2	P	168	VAL	2.3
2	R	227	ARG	2.3
2	G	181	LYS	2.3
2	L	264	LYS	2.3
2	B	27	TYR	2.3
3	X	178	TYR	2.3
1	1	192	GLN	2.3
2	Q	23	ASP	2.3
2	H	233	ILE	2.3
2	R	235	ILE	2.3
2	K	18	VAL	2.3
2	L	202	ASN	2.3
2	Q	182	ASN	2.3
2	I	207	TRP	2.3
2	Q	7	THR	2.3
2	N	246	ALA	2.3
2	Q	75	ALA	2.3
2	R	75	ALA	2.3
2	F	9	PHE	2.3
2	P	187	ILE	2.3
2	Q	226	GLY	2.3
1	Z	202	ASN	2.3
2	B	144	THR	2.3
1	1	39	CYS	2.3
2	E	220	LEU	2.3
1	Y	151	PHE	2.3
2	E	253	ILE	2.3
2	P	8	PHE	2.3
1	Y	314	SER	2.3
2	F	40	ARG	2.3
2	H	243	TRP	2.3
1	Y	316	SER	2.3
2	D	226	GLY	2.3
2	H	214	PRO	2.3
2	J	256	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	146	ASP	2.3
2	E	93	THR	2.2
2	F	229	THR	2.2
2	H	191	PHE	2.2
3	U	44	GLN	2.2
2	C	227	ARG	2.2
2	E	200	GLY	2.2
3	V	298	VAL	2.2
1	1	336	ASP	2.2
2	I	242	THR	2.2
2	M	58	THR	2.2
2	N	228	ASP	2.2
2	Q	185	LEU	2.2
2	Q	5	ASN	2.2
2	R	258	ASN	2.2
2	H	197	ILE	2.2
2	I	253	ILE	2.2
2	H	246	ALA	2.2
2	Q	246	ALA	2.2
2	R	62	ALA	2.2
1	1	263	TYR	2.2
2	Q	27	TYR	2.2
3	W	170	TYR	2.2
2	E	188	VAL	2.2
2	Q	168	VAL	2.2
1	Z	315	PRO	2.2
2	H	226	GLY	2.2
2	R	144	THR	2.2
2	H	253	ILE	2.2
2	H	263	ILE	2.2
2	M	263	ILE	2.2
1	1	291	LYS	2.2
2	H	264	LYS	2.2
3	T	43	TRP	2.2
2	G	29	MET	2.2
2	L	176	LEU	2.2
2	B	257	GLY	2.2
2	D	222	GLY	2.2
2	R	252	PRO	2.2
1	Y	318	ILE	2.2
2	I	235	ILE	2.2
2	L	142	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	I	183	ASN	2.2
2	J	258	ASN	2.2
2	E	201	TRP	2.2
2	P	225	ALA	2.2
3	U	168	TYR	2.2
2	E	168	VAL	2.2
3	T	275	GLU	2.2
2	I	206	THR	2.2
2	I	255	THR	2.2
2	R	264	LYS	2.2
2	H	228	ASP	2.2
2	Q	170	ALA	2.2
2	R	254	ALA	2.2
3	U	164	ALA	2.2
2	K	201	TRP	2.2
2	H	194	VAL	2.2
2	Q	18	VAL	2.2
2	Q	38	ILE	2.2
2	O	262	PHE	2.2
2	E	151	ASN	2.2
2	E	246	ALA	2.1
2	E	254	ALA	2.1
2	F	62	ALA	2.1
2	J	227	ARG	2.1
2	G	150	VAL	2.1
2	I	97	VAL	2.1
1	1	142	LYS	2.1
2	I	200	GLY	2.1
2	M	226	GLY	2.1
3	V	195	GLU	2.1
2	D	2	THR	2.1
2	Q	14	THR	2.1
2	R	48	ASN	2.1
3	U	41	ASN	2.1
3	X	46	ASN	2.1
2	N	141	GLN	2.1
2	O	260	SER	2.1
2	R	218	GLN	2.1
2	R	260	SER	2.1
3	T	44	GLN	2.1
2	E	187	ILE	2.1
2	I	34	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	184	ASP	2.1
1	Y	291	LYS	2.1
2	D	259	GLY	2.1
3	S	173	GLY	2.1
2	R	69	LEU	2.1
2	F	247	ASN	2.1
2	F	61	ILE	2.1
2	D	264	LYS	2.1
2	F	217	VAL	2.1
2	I	264	LYS	2.1
3	V	158	LYS	2.1
2	J	222	GLY	2.1
3	U	140	GLU	2.1
2	O	134	THR	2.1
2	R	256	ARG	2.1
2	F	215	ALA	2.1
2	E	219	SER	2.1
2	G	258	ASN	2.1
2	I	5	ASN	2.1
2	Q	88	ILE	2.1
2	M	67	PHE	2.1
3	S	50	VAL	2.1
2	B	200	GLY	2.1
2	D	176	LEU	2.1
3	T	122	GLY	2.1
3	U	178	TYR	2.1
3	W	219	ASP	2.1
2	E	96	PRO	2.1
2	M	187	ILE	2.1
2	P	254	ALA	2.1
2	E	260	SER	2.1
2	E	5	ASN	2.1
2	N	198	GLN	2.1
3	V	41	ASN	2.1
2	L	221	VAL	2.1
2	M	203	MET	2.1
3	W	47	GLY	2.1
1	Y	372	PRO	2.1
2	G	227	ARG	2.1
2	H	137	LYS	2.1
2	Q	253	ILE	2.1
2	R	159	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	S	172	LYS	2.1
2	O	246	ALA	2.1
2	F	53	VAL	2.1
2	K	5	ASN	2.1
2	F	178	LEU	2.1
2	G	168	VAL	2.1
2	I	217	VAL	2.1
2	Q	161	VAL	2.1
2	P	109	GLY	2.0
3	W	49	GLY	2.0
1	1	211	ARG	2.0
2	E	154	THR	2.0
2	J	160	ASP	2.0
2	R	2	THR	2.0
1	Z	125	ILE	2.0
1	Z	127	LYS	2.0
1	Z	156	ILE	2.0
2	H	4	LYS	2.0
2	R	60	ILE	2.0
3	T	172	LYS	2.0
1	1	13	ASN	2.0
1	Y	335	ASN	2.0
1	Z	242	ASN	2.0
2	A	109	GLY	2.0
2	N	63	GLY	2.0
2	N	78	GLY	2.0
2	H	211	PRO	2.0
2	N	137	LYS	2.0
2	A	49	THR	2.0
2	F	125	ILE	2.0
2	E	174	LEU	2.0
2	J	185	LEU	2.0
2	L	254	ALA	2.0
2	N	6	PHE	2.0
2	Q	143	SER	2.0
2	I	218	GLN	2.0
2	M	188	VAL	2.0
2	Q	217	VAL	2.0
2	H	5	ASN	2.0
3	X	49	GLY	2.0
2	H	3	ILE	2.0
1	1	257	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	1	320	THR	2.0
2	H	7	THR	2.0
2	F	224	PHE	2.0
2	H	201	TRP	2.0
2	M	68	GLU	2.0
2	E	149	SER	2.0
2	H	225	ALA	2.0
2	P	228	ASP	2.0
1	Y	319	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SR	V	1299	1/1	0.97	0.14	80,80,80,80	0
4	SR	W	1299	1/1	0.97	0.13	80,80,80,80	0
4	SR	U	1299	1/1	0.98	0.12	82,82,82,82	0
4	SR	S	1299	1/1	0.98	0.12	87,87,87,87	0
4	SR	T	1299	1/1	0.98	0.15	80,80,80,80	0
4	SR	X	1299	1/1	0.99	0.11	83,83,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.