



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:33 AM GMT

PDB ID : 2X53
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.; Vanheel, 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : trunk26765
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

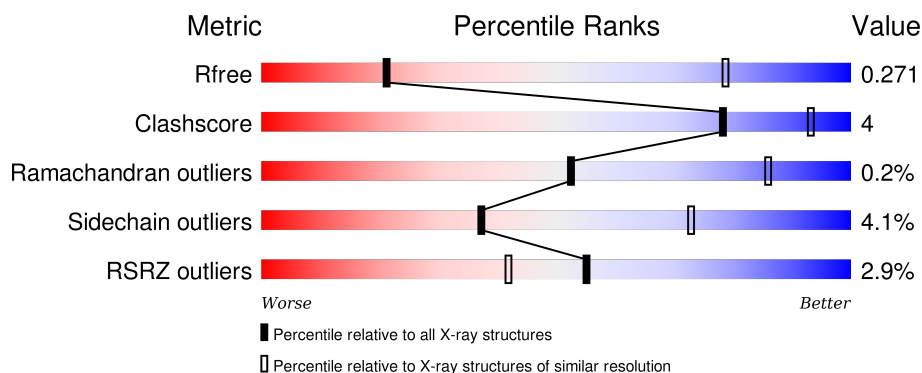
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.





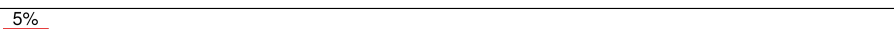
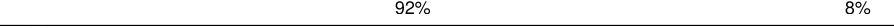


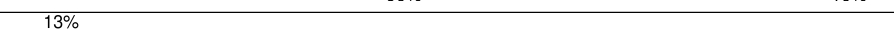



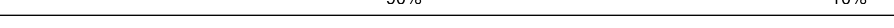


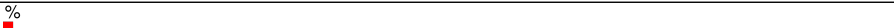
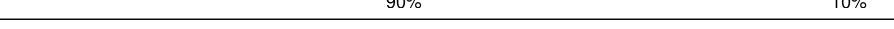


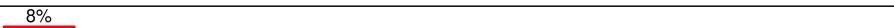




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	375	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	Y	375	<div> <div>%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	Z	375	<div> <div>%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
2	A	263	<div> <div>90%</div> <div>10%</div> </div>
2	B	263	<div> <div>92%</div> <div>8%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	263	
2	D	263	
2	E	263	
2	F	263	
2	G	263	
2	H	263	
2	I	263	
2	J	263	
2	K	263	
2	L	263	
2	M	263	
2	N	263	
2	O	263	
2	P	263	
2	Q	263	
2	R	263	
3	S	298	
3	T	298	
3	U	298	
3	V	298	
3	W	298	
3	X	298	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SR	V	1299	-	-	-	X

2 Entry composition

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
1	1	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	Y	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			
1	Z	372	Total	C	N	O	S	0	0	0
			3000	1918	493	581	8			

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is a protein called ORF15.

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

- Molecule 4 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

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

Continued on next page...

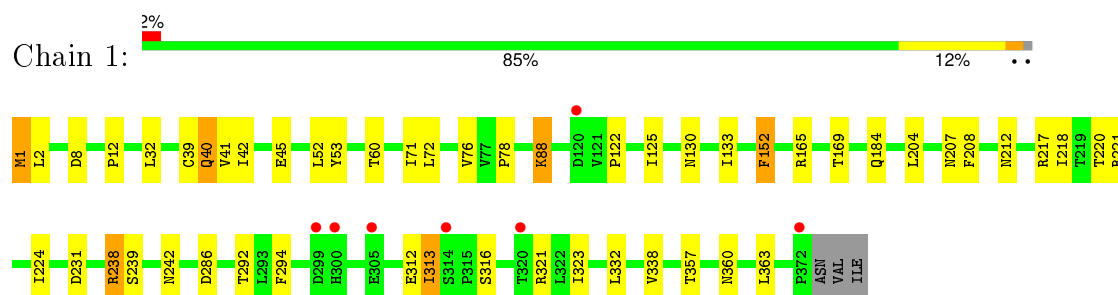
Continued from previous page...

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

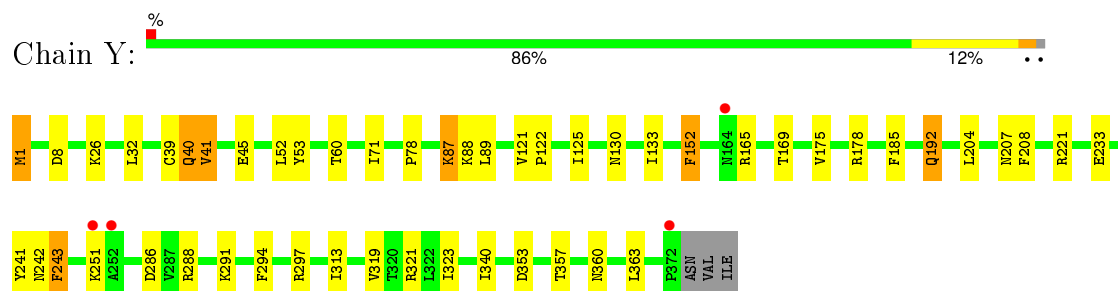
3 Residue-property plots

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.

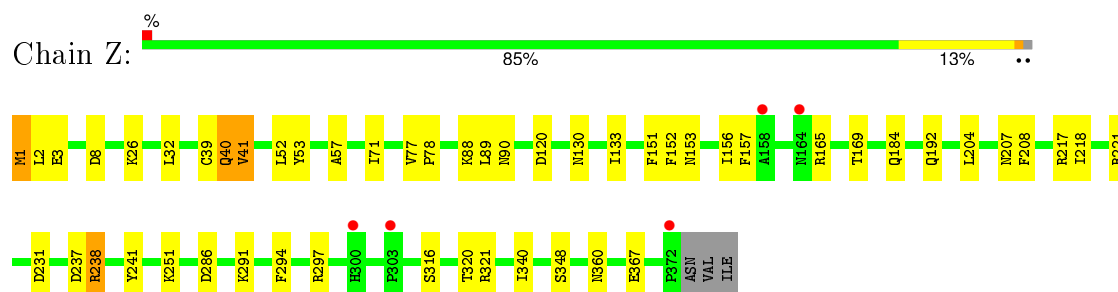
• Molecule 1: ORF16



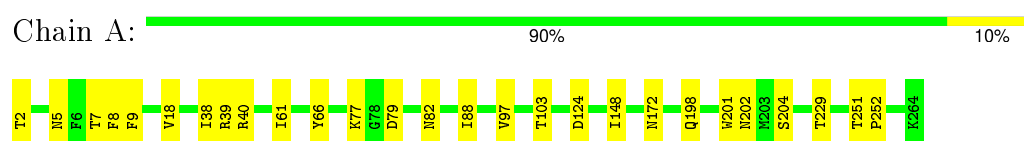
• Molecule 1: ORF16




• Molecule 1: ORF16



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



• Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain B: 



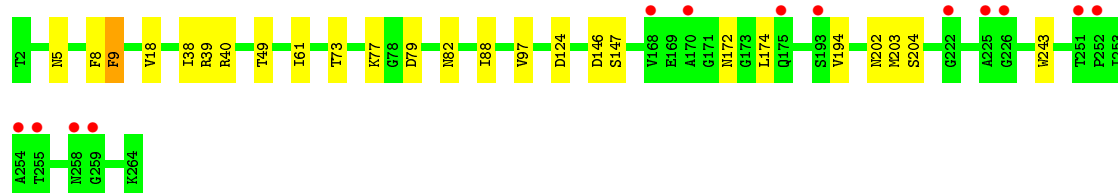
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain C: 



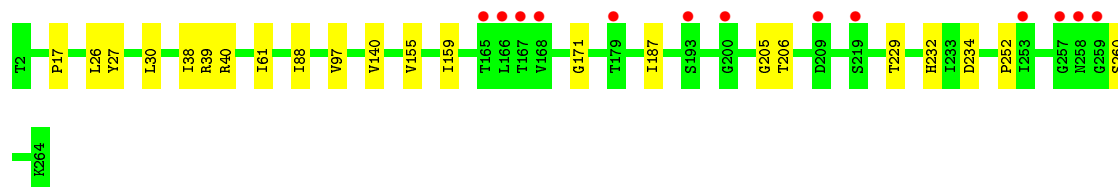
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain D: 



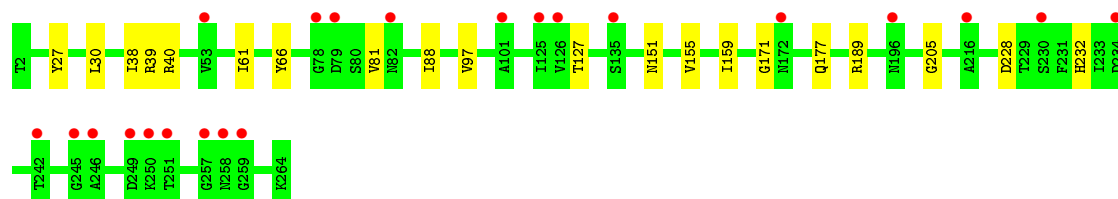
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain E: 

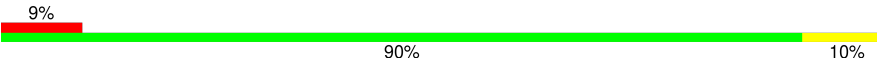


- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

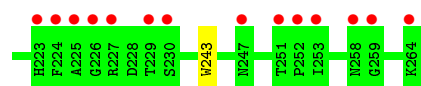
Chain F: 



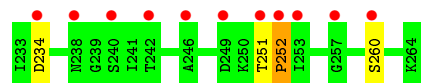
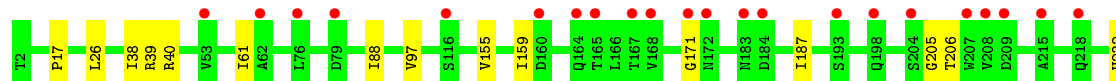
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain G: 

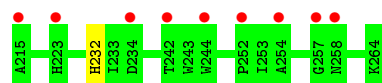
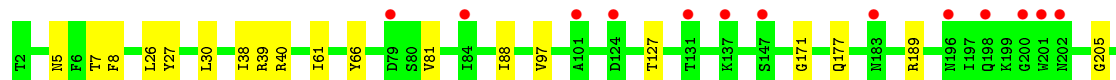




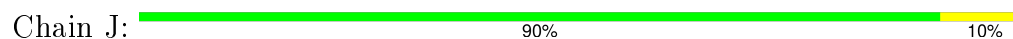
● Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN



● 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

Chain N: 92% 8%



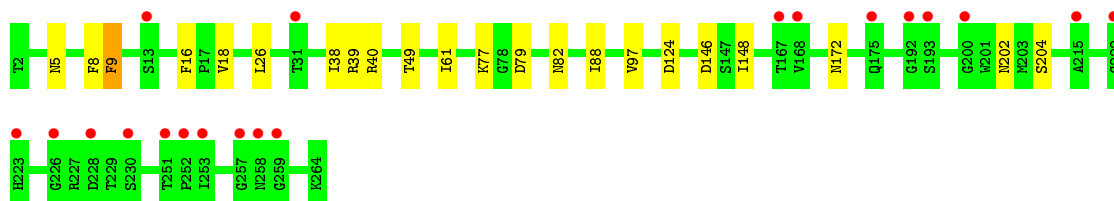
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain O: 92% 8%



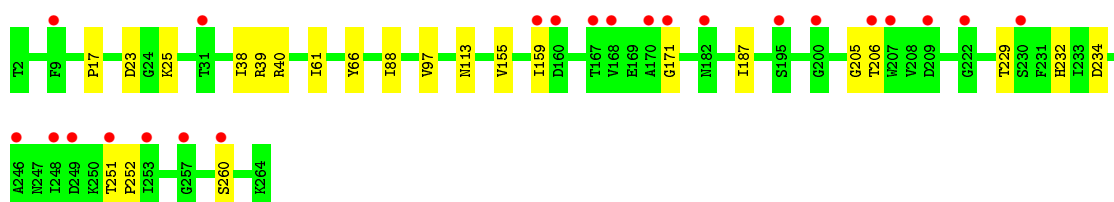
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain P: 8% 92% 8%



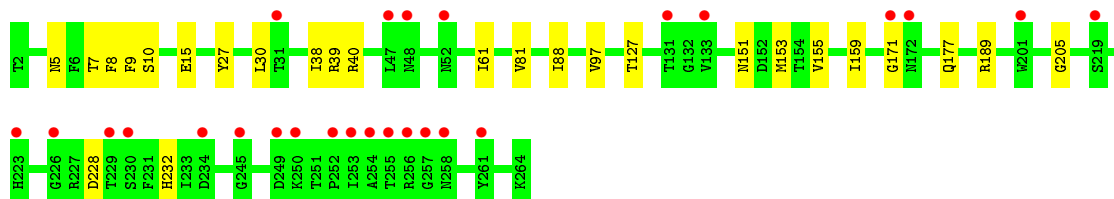
- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

Chain Q: 9% 91% 9%

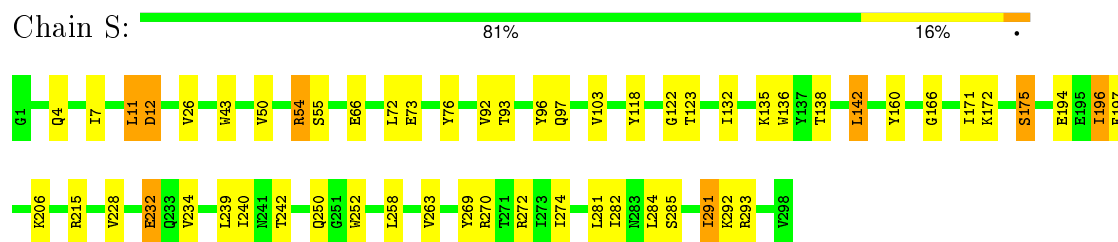


- Molecule 2: PUTATIVE RECEPTOR BINDING PROTEIN

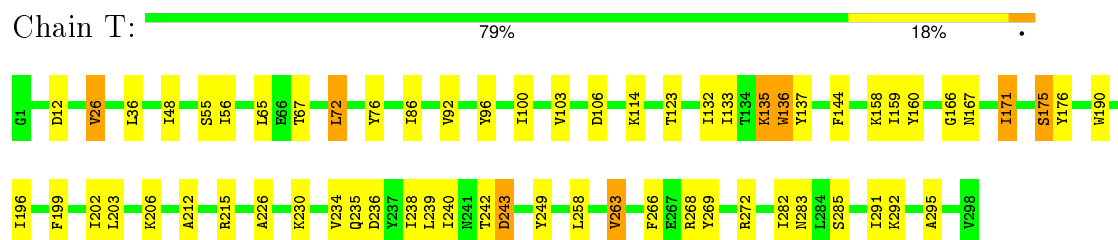
Chain R: 10% 90% 10%



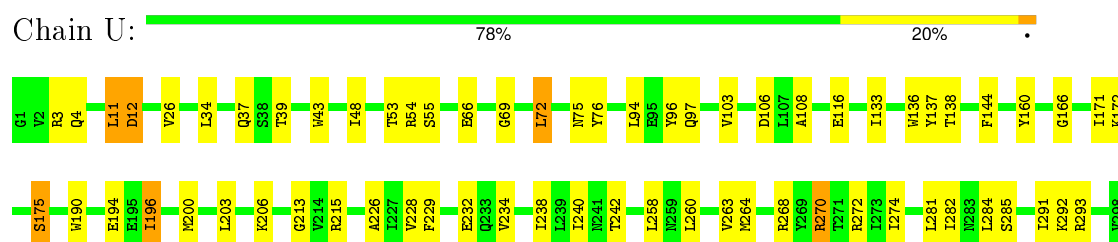
- Molecule 3: ORF15



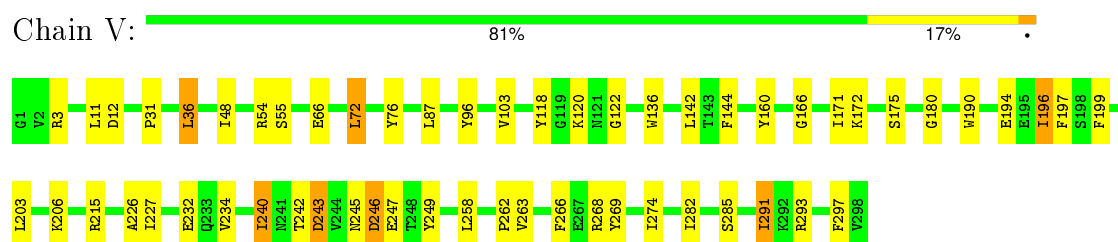
• Molecule 3: ORF15



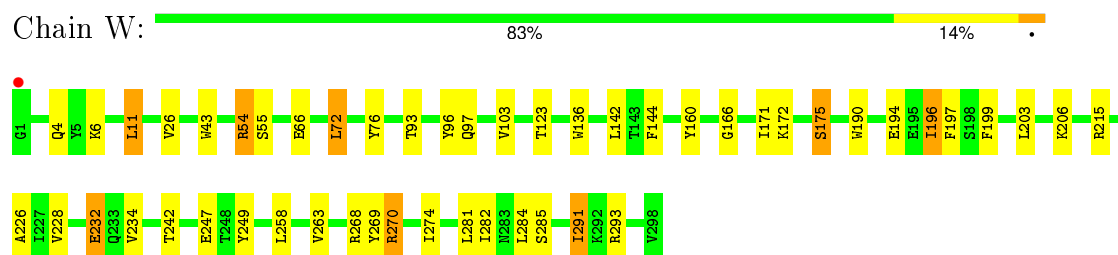
• Molecule 3: ORF15



• Molecule 3: ORF15

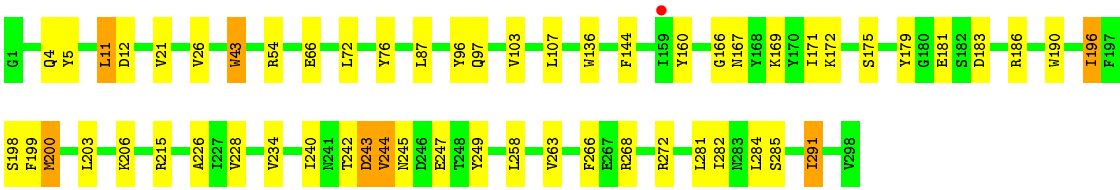


• Molecule 3: ORF15



• Molecule 3: ORF15





4 Data and refinement statistics

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 39.15 – 3.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (39.31-3.90) 96.9 (39.15-3.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.87Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.229 , 0.242 0.258 , 0.271	Depositor DCC
R_{free} test set	4219 reflections (2.99%)	DCC
Wilson B-factor (Å ²)	83.1	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 85.7	EDS
Estimated twinning fraction	0.010 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 141150 reflections	Xtriage
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

Xtriage'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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.38	0/3069	0.64	0/4175
1	Y	0.38	0/3069	0.65	0/4175
1	Z	0.38	0/3069	0.63	0/4175
2	A	0.32	0/2048	0.63	0/2791
2	B	0.36	0/2048	0.58	0/2791
2	C	0.35	0/2048	0.59	0/2791
2	D	0.32	0/2048	0.61	0/2791
2	E	0.36	0/2048	0.58	0/2791
2	F	0.36	0/2048	0.58	0/2791
2	G	0.32	0/2048	0.62	0/2791
2	H	0.37	0/2048	0.58	0/2791
2	I	0.37	0/2048	0.58	0/2791
2	J	0.34	0/2048	0.63	0/2791
2	K	0.36	0/2048	0.59	0/2791
2	L	0.36	0/2048	0.58	0/2791
2	M	0.34	0/2048	0.63	0/2791
2	N	0.36	0/2048	0.58	0/2791
2	O	0.36	0/2048	0.58	0/2791
2	P	0.34	0/2048	0.63	0/2791
2	Q	0.37	0/2048	0.58	0/2791
2	R	0.37	0/2048	0.59	0/2791
3	S	0.36	0/2485	0.69	0/3356
3	T	0.36	0/2485	0.69	0/3356
3	U	0.35	0/2485	0.67	0/3356
3	V	0.36	0/2485	0.67	0/3356
3	W	0.35	0/2485	0.66	0/3356
3	X	0.36	0/2485	0.67	0/3356
All	All	0.36	0/60981	0.62	0/82899

There are no bond length outliers.

There are no bond angle outliers.

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	35	0
1	Y	3000	0	2956	25	0
1	Z	3000	0	2956	32	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	34	0
3	T	2432	0	2394	35	0
3	U	2432	0	2394	35	0
3	V	2432	0	2394	28	0
3	W	2432	0	2394	23	0
3	X	2432	0	2394	40	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	59742	0	58710	423	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 (423) 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
3:S:242:THR:HG22	3:S:272:ARG:CG	2.22	0.69
2:P:77:LYS:H	2:P:82:ASN:HD21	1.41	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:Z:90:ASN:HD22	1:Z:192:GLN:NE2	1.99	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
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:U:116:GLU:HB2	3:V:31:PRO:HD2	1.85	0.59
3:S:206:LYS:HG3	3:S:285:SER:HB3	1.84	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
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
3:V:247:GLU:OE1	3:V:249:TYR:CE2	2.56	0.58
2:O:88:ILE:HG12	2:O:97:VAL:HG22	1.86	0.58
1:Z:153:ASN:HB3	1:Z:156:ILE:HG12	1.85	0.58
2:R:88:ILE:HG12	2:R:97:VAL:HG22	1.85	0.58
3:X:266:PHE:HB3	1:Y:221:ARG:HB2	1.85	0.58
2:I:88:ILE:HG12	2:I:97:VAL:HG22	1.85	0.58
3:V:226:ALA:HB3	3:V:268:ARG:HB3	1.85	0.58
1:Z:41:VAL:HG23	1:Z:57:ALA:HB1	1.85	0.58
2:F:88:ILE:HG12	2:F:97:VAL:HG22	1.86	0.58
3:X:206:LYS:HG3	3:X:285:SER:HB3	1.86	0.58
3:V:171:ILE:HG22	3:V:172:LYS:H	1.68	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:O	3:T:240:ILE:HD12	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
1:Z:41:VAL:HG11	1:Z:71:ILE:HG12	1.88	0.56
2:B:187:ILE:HG12	2:B:260:SER:HB3	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:O	3:U:240:ILE:HD12	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:88:ILE:HG12	2:N:97:VAL:HG22	1.89	0.55
2:E:187:ILE:HG12	2:E:260:SER:HB3	1.88	0.55
3:X:247:GLU:OE1	3:X:249:TYR:CE2	2.59	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
2:B:88:ILE:HG12	2:B:97:VAL:HG22	1.88	0.55
2:H:187:ILE:HG12	2:H:260:SER:HB3	1.88	0.55
2:E:88:ILE:HG12	2:E:97:VAL:HG22	1.89	0.55
1:1:221:ARG:HB2	3:V:266:PHE:HB3	1.87	0.55
2:P:5:ASN:HB3	2:P:8:PHE:CD1	2.42	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
1:Y:243:PHE:C	1:Y:243:PHE:CD1	2.80	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: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:X:226:ALA:HB3	3:X:268:ARG:HB3	1.89	0.53
3:V:142:LEU:HG	3:V:291:ILE:HD12	1.90	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
3:T:215:ARG:HB3	3:T:282:ILE:HD11	1.90	0.53
2:P:26:LEU:HD13	2:Q:66:TYR:HB2	1.91	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
2:L:145:LEU:HD13	2:L:148:ILE:HD11	1.91	0.53
1:1:45:GLU:HA	1:1:357:THR:HG22	1.91	0.53
3:W:196:ILE:HG13	3:W:274:ILE:HB	1.90	0.52
2:Q:25:LYS:HE2	2:Q:113:ASN:HB3	1.91	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:T:206:LYS:HG3	3:T:285:SER:HB3	1.91	0.52
3:T:132:ILE:HD13	3:T:135:LYS:HG3	1.92	0.52
2:J:88:ILE:HG12	2:J:97:VAL:HG22	1.90	0.52
3:W:226:ALA:HB3	3:W:268:ARG:HB3	1.92	0.52
2:A:5:ASN:HB3	2:A:8:PHE:CD1	2.44	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
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:U:138:THR:O	3:U:292:LYS:HA	2.11	0.51
3:T:199:PHE:H	3:T:242:THR:HG1	1.57	0.51
3:T:199:PHE:N	3:T:242:THR:OG1	2.39	0.50
3:V:240:ILE:C	3:V:240:ILE:HD12	2.32	0.50
2:O:177:GLN:HB3	2:O:189:ARG:HB2	1.93	0.50
2:C:177:GLN:HB3	2:C:189:ARG:HB2	1.93	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
3:T:243:ASP:OD1	3:T:243:ASP:C	2.50	0.50
2:A:148:ILE:HB	2:C:153:MET:HG3	1.92	0.50
2:P:5:ASN:O	2:P:16:PHE:HB3	2.11	0.50
2:J:26:LEU:HD13	2:K:66:TYR:HB2	1.94	0.50
2:A:172:ASN:HD21	2:A:204:SER:H	1.60	0.50
1:I:32:LEU:HD11	1:I:204:LEU:HB2	1.93	0.50
2:O:171:GLY:HA3	2:O:205:GLY:H	1.77	0.50
3:V:96:TYR:HB3	3:V:103:VAL:HG23	1.94	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
2:L:171:GLY:HA3	2:L:205:GLY:H	1.77	0.50
3:X:167:ASN:HD22	3:X:169:LYS:HE3	1.76	0.50
3:S:11:LEU:O	3:S:12:ASP:CG	2.51	0.50
2:Q:39:ARG:HB2	2:Q:61:ILE:HB	1.94	0.50
2:D:88:ILE:HG12	2:D:97:VAL:HG22	1.93	0.50
2:F:171:GLY:HA3	2:F:205:GLY:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:196:ILE:HG13	3:U:274:ILE:HB	1.94	0.49
3:W:4:GLN:HB2	3:W:97:GLN:HB3	1.94	0.49
3:S:171:ILE:HG22	3:S:172:LYS:H	1.76	0.49
3:U:281:LEU:HB3	3:U:284:LEU:HD12	1.92	0.49
3:X:199:PHE:CZ	3:X:242:THR:HG21	2.47	0.49
2:R:177:GLN:HB3	2:R:189:ARG:HB2	1.93	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:F:177:GLN:HB3	2:F:189:ARG:HB2	1.93	0.49
1:1:122:PRO:HD2	1:1:125:ILE:HD12	1.94	0.49
1:Y:39:CYS:HB2	1:Y:60:THR:OG1	2.12	0.49
2:J:5:ASN:HB3	2:J:8:PHE:CD1	2.47	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
2:H:39:ARG:HB2	2:H:61:ILE:HB	1.94	0.49
1:1:218:ILE:HB	1:1:338:VAL:HG12	1.95	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
1:1:242:ASN:O	1:1:313:ILE:HD12	2.12	0.49
1:1:184:GLN:HE22	1:1:217:ARG:HH22	1.61	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
1:Z:152:PHE:CB	1:Z:208:PHE:HB2	2.42	0.49
2:B:39:ARG:HB2	2:B:61:ILE:HB	1.95	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
1:Z:237:ASP:C	1:Z:238:ARG:HG2	2.33	0.48
3:U:194:GLU:HB2	3:U:293:ARG:HD2	1.96	0.48
2:E:39:ARG:HB2	2:E:61:ILE:HB	1.94	0.48
3:U:171:ILE:HG22	3:U:172:LYS:H	1.77	0.48
2:I:27:TYR:HA	2:I:30:LEU:HD12	1.96	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:V:243:ASP:C	3:V:243:ASP:OD1	2.52	0.48
3:S:242:THR:O	3:S:272:ARG:HD3	2.14	0.48
3:X:281:LEU:HB3	3:X:284:LEU:HD12	1.96	0.48
3:V:36:LEU:HD21	3:V:297:PHE:HB2	1.96	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:T:199:PHE:CE1	3:T:242:THR:HG21	2.48	0.48
3:X:4:GLN:HB2	3:X:97:GLN:HB3	1.96	0.48
1:1:231:ASP:OD2	1:1:321:ARG:NH1	2.47	0.48
3:W:11:LEU:HD12	3:W:93:THR:HG21	1.96	0.48
3:S:239:LEU:C	3:S:239:LEU:HD23	2.34	0.48
3:V:144:PHE:HB3	3:V:190:TRP:CE2	2.49	0.48
3:T:26:VAL:HG23	3:T:67:THR:HG22	1.96	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
3:U:11:LEU:O	3:U:12:ASP:CG	2.52	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:172:ASN:HD21	2:P:204:SER:H	1.63	0.47
2:P:148:ILE:HB	2:R:153:MET:HG3	1.96	0.47
1:Y:45:GLU:HA	1:Y:357:THR:HG22	1.95	0.47
3:S:281:LEU:HB3	3:S:284:LEU:HD12	1.96	0.47
3:U:4:GLN:HB2	3:U:97:GLN:HB3	1.97	0.47
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
2:M:172:ASN:HD21	2:M:204:SER:H	1.62	0.46
1:1:42:ILE:HD13	3:X:43:TRP:NE1	2.30	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:V:160:TYR:HB3	3:V:166:GLY:HA3	1.95	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
3:V:196:ILE:HG22	3:V:293:ARG:HD3	1.98	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:N:171:GLY:HA3	2:N:205:GLY:H	1.81	0.46
1:Y:251:LYS:HG2	1:Y:297:ARG:HD3	1.97	0.46
2:M:148:ILE:HB	2:O:153:MET:HG3	1.98	0.46
3:S:72:LEU:HD22	3:S:76:TYR:CE2	2.50	0.46
3:U:272:ARG:NH1	1:Z:3:GLU:OE1	2.49	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
2:B:171:GLY:HA3	2:B:205:GLY:H	1.81	0.46
3:U:206:LYS:HG3	3:U:285:SER:HB3	1.98	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
2:D:172:ASN:HD21	2:D:204:SER:H	1.64	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
3:T:72:LEU:HD22	3:T:76:TYR:CE2	2.51	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:T:242:THR:O	3:T:272:ARG:HD3	2.16	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:X:96:TYR:HB3	3:X:103:VAL:HG23	1.98	0.45
3:T:240:ILE:HG22	3:T:249:TYR:HD1	1.82	0.45
2:J:172:ASN:HD21	2:J:204:SER:H	1.63	0.45
1:Y:130:ASN:HA	1:Y:133:ILE:HD12	1.99	0.45
2:M:66:TYR:HB2	2:O:26:LEU:HD13	1.99	0.45
2:G:172:ASN:HD21	2:G:204:SER:H	1.63	0.45
2:B:26:LEU:HD13	2:C:66:TYR:HB2	1.99	0.45
3:W:144:PHE:HB3	3:W:190:TRP:CE2	2.52	0.45
3:U:229:PHE:CE1	3:U:264:MET:HB3	2.52	0.45
3:T:266:PHE:HB3	1:Z:221:ARG:HB2	1.99	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
3:U:96:TYR:HB3	3:U:103:VAL:HG23	1.99	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
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:C:81:VAL:HG22	2:C:127:THR:HG23	1.99	0.44
1:Z:251:LYS:HG2	1:Z:297:ARG:HD3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:66:TYR:HB2	2:C:26:LEU:HD13	1.99	0.44
2:H:171:GLY:HA3	2:H:205:GLY:H	1.81	0.44
2:E:26:LEU:HD13	2:F:66:TYR:HB2	1.98	0.44
1:Z:1:MET:HG3	1:Z:40:GLN:HB2	2.00	0.44
3:U:144:PHE:HB3	3:U:190:TRP:CE2	2.52	0.44
2:R:9:PHE:HZ	3:X:181:GLU:HG3	1.73	0.44
2:J:77:LYS:H	2:J:82:ASN:ND2	2.12	0.44
3:V:194:GLU:HB2	3:V:293:ARG:HD2	1.99	0.44
1:I:220:THR:HG21	1:I:332:LEU:HD21	2.00	0.44
2:J:251:THR:HA	2:J:252:PRO:HD3	1.87	0.44
3:U:229:PHE:CD1	3:U:260:LEU:HB3	2.52	0.44
2:O:81:VAL:HG22	2:O:127:THR:HG23	1.99	0.44
1:Z:32:LEU:HD11	1:Z:204:LEU:HB2	1.99	0.44
2:F:39:ARG:HB2	2:F:61:ILE:HB	2.00	0.44
3:S:138:THR:O	3:S:292:LYS:HA	2.17	0.44
2:L:81:VAL:HG22	2:L:127:THR:HG23	2.00	0.44
3:T:136:TRP:HB2	3:T:295:ALA:O	2.17	0.44
2:G:9:PHE:HA	3:U:160:TYR:HB2	2.00	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
1:I:72:LEU:HD22	3:W:270:ARG:NH1	2.33	0.44
2:K:251:THR:HA	2:K:252:PRO:HD3	1.90	0.44
2:K:26:LEU:HD13	2:L:66:TYR:HB2	2.00	0.44
2:A:172:ASN:ND2	2:A:204:SER:H	2.16	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
3:S:96:TYR:HB3	3:S:103:VAL:HG23	1.99	0.44
2:C:39:ARG:HB2	2:C:61:ILE:HB	2.00	0.44
2:G:77:LYS:H	2:G:82:ASN:ND2	2.12	0.44
3:X:198:SER:HA	3:X:242:THR:OG1	2.18	0.44
3:S:239:LEU:HD23	3:S:240:ILE:N	2.32	0.44
3:W:247:GLU:OE1	3:W:249:TYR:HE2	2.01	0.44
2:D:39:ARG:HB2	2:D:61:ILE:HB	2.00	0.43
2:O:27:TYR:HA	2:O:30:LEU:HD12	2.00	0.43
2:F:81:VAL:HG22	2:F:127:THR:HG23	1.99	0.43
2:E:17:PRO:CB	3:T:167:ASN:HB2	2.48	0.43
2:D:146:ASP:O	2:F:151:ASN:HB2	2.17	0.43
2:D:73:THR:HG21	3:S:258:LEU:HD21	2.00	0.43
3:X:5:TYR:HB3	3:X:21:VAL:HG23	2.00	0.43
2:J:148:ILE:HB	2:L:153:MET:HG3	1.99	0.43
2:I:81:VAL:HG22	2:I:127:THR:HG23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:39:ARG:HB2	2:M:61:ILE:HB	2.00	0.43
3:U:203:LEU:HB2	3:U:238:ILE:HB	2.01	0.43
2:R:39:ARG:HB2	2:R:61:ILE:HB	2.00	0.43
3:S:132:ILE:HG21	3:S:135:LYS:HB2	2.00	0.43
1:Z:184:GLN:HE22	1:Z:217:ARG:HH22	1.66	0.43
3:T:202:ILE:HG12	3:T:239:LEU:HD12	2.01	0.43
2:O:155:VAL:HG21	2:O:159:ILE:HD11	2.01	0.43
3:X:196:ILE:HD11	3:X:199:PHE:HD1	1.84	0.43
1:I:39:CYS:HB2	1:I:60:THR:OG1	2.18	0.43
2:A:39:ARG:HB2	2:A:61:ILE:HB	2.00	0.43
3:U:242:THR:CG2	3:U:272:ARG:CG	2.93	0.43
2:P:77:LYS:H	2:P:82:ASN:ND2	2.12	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:O:39:ARG:HB2	2:O:61:ILE:HB	2.00	0.43
2:G:203:MET:SD	2:G:243:TRP:HB2	2.59	0.43
3:U:270:ARG:NH2	1:Z:90:ASN:HB3	2.33	0.43
2:G:39:ARG:HB2	2:G:61:ILE:HB	2.00	0.43
3:T:137:TYR:CE1	3:T:292:LYS:HD2	2.54	0.43
2:Q:155:VAL:HG21	2:Q:159:ILE:HD11	2.01	0.43
2:O:5:ASN:HB3	2:O:8:PHE:CD1	2.54	0.43
2:I:39:ARG:HB2	2:I:61:ILE:HB	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
1:I:1:MET:HG3	1:I:40:GLN:HB2	2.00	0.43
3:X:243:ASP:OD1	3:X:245:ASN:N	2.52	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
1:Y:52:LEU:HD23	1:Y:53:TYR:CE2	2.55	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:W:247:GLU:OE1	3:W:249:TYR:CE2	2.73	0.42
3:W:199:PHE:CE1	3:W:242:THR:HG21	2.55	0.42
2:G:174:LEU:HB2	2:G:194:VAL:HG22	2.02	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
3:U:226:ALA:HB3	3:U:268:ARG:HB3	2.01	0.42
2:H:251:THR:HA	2:H:252:PRO:HD3	1.89	0.42
2:B:251:THR:HA	2:B:252:PRO:HD3	1.93	0.42
2:I:5:ASN:HB3	2:I:8:PHE:CD1	2.55	0.42
3:W:196:ILE:HD13	3:W:291:ILE:HG12	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:155:VAL:HG21	2:C:159:ILE:HD11	2.02	0.42
1:1:12:PRO:HB2	1:Y:288:ARG:CZ	2.49	0.42
2:D:77:LYS:H	2:D:82:ASN:ND2	2.12	0.42
1:Y:121:VAL:HG11	1:Y:175:VAL:HG21	2.01	0.42
3:T:171:ILE:H	3:T:175:SER:HA	1.84	0.42
1:1:323:ILE:HA	1:1:363:LEU:O	2.20	0.42
1:Z:77:VAL:O	1:Z:89:LEU:HB3	2.20	0.41
2:M:5:ASN:O	2:M:16:PHE:HB3	2.20	0.41
2:L:39:ARG:HB2	2:L:61:ILE:HB	2.00	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
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:J:203:MET:SD	2:J:243:TRP:HB2	2.60	0.41
2:G:66:TYR:HB2	2:I:26:LEU:HD13	2.02	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:V:118:TYR:HB3	3:V:122:GLY:HA2	2.02	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:U:203:LEU:HD13	3:U:213:GLY:HA2	2.01	0.41
1:Z:241:TYR:CD2	1:Z:241:TYR:N	2.88	0.41
3:V:199:PHE:CZ	3:V:242:THR:HG21	2.55	0.41
1:1:52:LEU:HD23	1:1:53:TYR:CE2	2.56	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
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:G:5:ASN:HB3	2:G:8:PHE:CD1	2.56	0.41
1:1:294:PHE:CE2	1:Z:169:THR:CG2	3.03	0.41
1:1:76:VAL:HG21	1:1:88:LYS:HE3	2.02	0.41
2:N:155:VAL:HG21	2:N:159:ILE:HD11	2.01	0.41
3:T:158:LYS:HD2	3:T:176:TYR:CE1	2.56	0.41
2:P:146:ASP:O	2:R:151:ASN:HB2	2.21	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:Y:87:LYS:HZ1	1:Y:89:LEU:HD23	1.86	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
2:P:172:ASN:ND2	2:P:204:SER:H	2.19	0.40
1:Y:175:VAL:HG12	1:Y:178:ARG:HH12	1.86	0.40
3:V:246:ASP:O	3:V:246:ASP:CG	2.59	0.40
2:J:174:LEU:HB2	2:J:194:VAL:HG22	2.04	0.40
2:M:172:ASN:ND2	2:M:204:SER:H	2.19	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:E:229:THR:HB	2:F:228:ASP:HB2	2.03	0.40
3:V:240:ILE:CD1	3:V:242:THR:HG23	2.51	0.40
2:B:229:THR:HB	2:C:228:ASP:HB2	2.03	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
1:Y:185:PHE:CE2	1:Y:208:PHE:HA	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

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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	26	70
3	T	296/298 (99%)	273 (92%)	21 (7%)	2 (1%)	26	70
3	U	296/298 (99%)	274 (93%)	20 (7%)	2 (1%)	26	70
3	V	296/298 (99%)	275 (93%)	19 (6%)	2 (1%)	26	70
3	W	296/298 (99%)	280 (95%)	14 (5%)	2 (1%)	26	70
3	X	296/298 (99%)	277 (94%)	17 (6%)	2 (1%)	26	70
All	All	7584/7647 (99%)	7207 (95%)	365 (5%)	12 (0%)	52	86

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	324 (96%)	13 (4%)	39	74
1	Y	337/340 (99%)	319 (95%)	18 (5%)	28	67
1	Z	337/340 (99%)	321 (95%)	16 (5%)	32	70
2	A	227/227 (100%)	218 (96%)	9 (4%)	38	73
2	B	227/227 (100%)	221 (97%)	6 (3%)	54	81
2	C	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	D	227/227 (100%)	220 (97%)	7 (3%)	47	78
2	E	227/227 (100%)	221 (97%)	6 (3%)	54	81
2	F	227/227 (100%)	224 (99%)	3 (1%)	76	89
2	G	227/227 (100%)	219 (96%)	8 (4%)	43	76
2	H	227/227 (100%)	220 (97%)	7 (3%)	47	78
2	I	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	J	227/227 (100%)	219 (96%)	8 (4%)	43	76
2	K	227/227 (100%)	221 (97%)	6 (3%)	54	81
2	L	227/227 (100%)	223 (98%)	4 (2%)	66	87
2	M	227/227 (100%)	219 (96%)	8 (4%)	43	76
2	N	227/227 (100%)	221 (97%)	6 (3%)	54	81
2	O	227/227 (100%)	224 (99%)	3 (1%)	76	89
2	P	227/227 (100%)	220 (97%)	7 (3%)	47	78

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Q	227/227 (100%)	220 (97%)	7 (3%)	47	78
2	R	227/227 (100%)	223 (98%)	4 (2%)	66	87
3	S	264/264 (100%)	246 (93%)	18 (7%)	20	59
3	T	264/264 (100%)	247 (94%)	17 (6%)	22	61
3	U	264/264 (100%)	241 (91%)	23 (9%)	13	49
3	V	264/264 (100%)	241 (91%)	23 (9%)	13	49
3	W	264/264 (100%)	244 (92%)	20 (8%)	16	55
3	X	264/264 (100%)	247 (94%)	17 (6%)	22	61
All	All	6681/6690 (100%)	6409 (96%)	272 (4%)	37	73

All (272) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	1	MET
1	1	2	LEU
1	1	8	ASP
1	1	40	GLN
1	1	88	LYS
1	1	152	PHE
1	1	165	ARG
1	1	207	ASN
1	1	224	ILE
1	1	238	ARG
1	1	286	ASP
1	1	313	ILE
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	40	ARG
2	A	79	ASP
2	A	124	ASP
2	A	202	ASN
2	B	38	ILE
2	B	40	ARG
2	B	206	THR
2	B	232	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	234	ASP
2	B	252	PRO
2	C	7	THR
2	C	38	ILE
2	C	40	ARG
2	C	232	HIS
2	D	9	PHE
2	D	18	VAL
2	D	38	ILE
2	D	40	ARG
2	D	79	ASP
2	D	124	ASP
2	D	202	ASN
2	E	38	ILE
2	E	40	ARG
2	E	206	THR
2	E	232	HIS
2	E	234	ASP
2	E	252	PRO
2	F	38	ILE
2	F	40	ARG
2	F	232	HIS
2	G	7	THR
2	G	9	PHE
2	G	18	VAL
2	G	38	ILE
2	G	40	ARG
2	G	79	ASP
2	G	124	ASP
2	G	202	ASN
2	H	17	PRO
2	H	38	ILE
2	H	40	ARG
2	H	206	THR
2	H	232	HIS
2	H	234	ASP
2	H	252	PRO
2	I	7	THR
2	I	38	ILE
2	I	40	ARG
2	I	232	HIS
2	J	7	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	9	PHE
2	J	18	VAL
2	J	38	ILE
2	J	40	ARG
2	J	79	ASP
2	J	124	ASP
2	J	202	ASN
2	K	23	ASP
2	K	38	ILE
2	K	40	ARG
2	K	206	THR
2	K	232	HIS
2	K	234	ASP
2	L	26	LEU
2	L	38	ILE
2	L	40	ARG
2	L	232	HIS
2	M	7	THR
2	M	9	PHE
2	M	18	VAL
2	M	38	ILE
2	M	40	ARG
2	M	79	ASP
2	M	124	ASP
2	M	202	ASN
2	N	23	ASP
2	N	38	ILE
2	N	40	ARG
2	N	206	THR
2	N	232	HIS
2	N	234	ASP
2	O	38	ILE
2	O	40	ARG
2	O	232	HIS
2	P	9	PHE
2	P	18	VAL
2	P	38	ILE
2	P	40	ARG
2	P	79	ASP
2	P	124	ASP
2	P	202	ASN
2	Q	17	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	Q	23	ASP
2	Q	38	ILE
2	Q	40	ARG
2	Q	206	THR
2	Q	232	HIS
2	Q	234	ASP
2	R	7	THR
2	R	38	ILE
2	R	40	ARG
2	R	232	HIS
3	S	11	LEU
3	S	12	ASP
3	S	26	VAL
3	S	43	TRP
3	S	54	ARG
3	S	55	SER
3	S	66	GLU
3	S	123	THR
3	S	142	LEU
3	S	196	ILE
3	S	197	PHE
3	S	228	VAL
3	S	232	GLU
3	S	234	VAL
3	S	263	VAL
3	S	269	TYR
3	S	270	ARG
3	S	291	ILE
3	T	12	ASP
3	T	26	VAL
3	T	48	ILE
3	T	55	SER
3	T	65	LEU
3	T	72	LEU
3	T	123	THR
3	T	135	LYS
3	T	159	ILE
3	T	171	ILE
3	T	196	ILE
3	T	203	LEU
3	T	234	VAL
3	T	236	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	T	243	ASP
3	T	263	VAL
3	T	269	TYR
3	U	3	ARG
3	U	11	LEU
3	U	12	ASP
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	66	GLU
3	U	72	LEU
3	U	94	LEU
3	U	196	ILE
3	U	200	MET
3	U	228	VAL
3	U	232	GLU
3	U	234	VAL
3	U	258	LEU
3	U	263	VAL
3	U	270	ARG
3	U	291	ILE
3	V	3	ARG
3	V	11	LEU
3	V	12	ASP
3	V	36	LEU
3	V	48	ILE
3	V	54	ARG
3	V	55	SER
3	V	66	GLU
3	V	72	LEU
3	V	120	LYS
3	V	196	ILE
3	V	197	PHE
3	V	203	LEU
3	V	227	ILE
3	V	232	GLU
3	V	234	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	V	240	ILE
3	V	243	ASP
3	V	246	ASP
3	V	258	LEU
3	V	263	VAL
3	V	269	TYR
3	V	291	ILE
3	W	6	LYS
3	W	11	LEU
3	W	26	VAL
3	W	43	TRP
3	W	54	ARG
3	W	55	SER
3	W	66	GLU
3	W	72	LEU
3	W	123	THR
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	258	LEU
3	W	263	VAL
3	W	269	TYR
3	W	270	ARG
3	W	291	ILE
3	X	11	LEU
3	X	26	VAL
3	X	43	TRP
3	X	54	ARG
3	X	66	GLU
3	X	107	LEU
3	X	179	TYR
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	X	263	VAL
3	X	291	ILE
1	Y	1	MET
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	152	PHE
1	Y	165	ARG
1	Y	192	GLN
1	Y	207	ASN
1	Y	242	ASN
1	Y	243	PHE
1	Y	286	ASP
1	Y	319	VAL
1	Y	340	ILE
1	Y	353	ASP
1	Y	360	ASN
1	Z	1	MET
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	151	PHE
1	Z	165	ARG
1	Z	207	ASN
1	Z	238	ARG
1	Z	286	ASP
1	Z	320	THR
1	Z	340	ILE
1	Z	360	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	184	GLN
1	1	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	5	ASN
2	A	71	ASN
2	A	82	ASN
2	A	92	GLN
2	A	172	ASN
2	A	175	GLN
2	A	196	ASN
2	B	71	ASN
2	C	172	ASN
2	D	5	ASN
2	D	71	ASN
2	D	82	ASN
2	D	92	GLN
2	D	172	ASN
2	D	175	GLN
2	D	196	ASN
2	E	54	GLN
2	E	71	ASN
2	F	172	ASN
2	G	71	ASN
2	G	82	ASN
2	G	92	GLN
2	G	172	ASN
2	G	175	GLN
2	G	196	ASN
2	H	71	ASN
2	I	151	ASN
2	I	172	ASN
2	J	71	ASN
2	J	82	ASN
2	J	172	ASN
2	J	175	GLN
2	J	196	ASN
2	K	71	ASN
2	L	151	ASN
2	L	172	ASN
2	M	71	ASN
2	M	82	ASN
2	M	172	ASN
2	M	175	GLN
2	M	196	ASN
2	N	71	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	172	ASN
2	P	5	ASN
2	P	71	ASN
2	P	82	ASN
2	P	92	GLN
2	P	172	ASN
2	P	175	GLN
2	P	196	ASN
2	Q	54	GLN
2	Q	71	ASN
2	R	172	ASN
3	S	102	GLN
3	S	250	GLN
3	T	102	GLN
3	T	167	ASN
3	T	235	GLN
3	U	23	ASN
3	U	75	ASN
3	U	250	GLN
3	V	23	ASN
3	V	102	GLN
3	V	250	GLN
3	W	102	GLN
3	X	102	GLN
3	X	167	ASN
3	X	250	GLN
1	Y	90	ASN
1	Y	143	ASN
1	Z	143	ASN
1	Z	184	GLN
1	Z	192	GLN

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

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

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 ⓘ

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%)	0.19	7 (1%) 70 59	63, 97, 170, 239	0
1	Y	372/375 (99%)	0.07	4 (1%) 82 74	62, 94, 151, 270	0
1	Z	372/375 (99%)	0.15	5 (1%) 79 70	63, 98, 166, 246	0
2	A	263/263 (100%)	-0.13	0 100 100	44, 76, 105, 140	0
2	B	263/263 (100%)	-0.01	1 (0%) 93 90	55, 88, 126, 147	0
2	C	263/263 (100%)	0.05	1 (0%) 93 90	55, 90, 137, 172	0
2	D	263/263 (100%)	0.27	13 (4%) 33 24	52, 106, 248, 290	0
2	E	263/263 (100%)	0.44	13 (4%) 33 24	64, 121, 259, 286	0
2	F	263/263 (100%)	0.51	22 (8%) 14 9	57, 144, 245, 291	0
2	G	263/263 (100%)	0.40	24 (9%) 11 8	60, 126, 249, 285	0
2	H	263/263 (100%)	0.80	33 (12%) 5 5	97, 155, 233, 282	0
2	I	263/263 (100%)	0.72	22 (8%) 14 9	75, 156, 262, 297	0
2	J	263/263 (100%)	0.07	1 (0%) 93 90	55, 102, 163, 246	0
2	K	263/263 (100%)	0.07	0 100 100	52, 84, 175, 233	0
2	L	263/263 (100%)	0.11	1 (0%) 93 90	62, 102, 162, 220	0
2	M	263/263 (100%)	0.21	2 (0%) 87 81	76, 126, 166, 208	0
2	N	263/263 (100%)	0.06	0 100 100	60, 95, 142, 163	0
2	O	263/263 (100%)	0.26	0 100 100	85, 128, 168, 184	0
2	P	263/263 (100%)	0.47	20 (7%) 17 11	65, 132, 296, 298	0
2	Q	263/263 (100%)	0.74	23 (8%) 13 9	96, 154, 288, 292	0
2	R	263/263 (100%)	0.75	26 (9%) 9 7	83, 160, 292, 300	0
3	S	298/298 (100%)	-0.24	0 100 100	41, 64, 106, 124	0
3	T	298/298 (100%)	-0.29	0 100 100	42, 65, 113, 145	0
3	U	298/298 (100%)	-0.19	0 100 100	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%)	-0.22	0 100 100	44, 66, 101, 127	0
3	W	298/298 (100%)	-0.18	1 (0%) 94 91	40, 67, 132, 161	0
3	X	298/298 (100%)	-0.17	1 (0%) 94 91	40, 67, 158, 202	0
All	All	7638/7647 (99%)	0.17	220 (2%) 55 42	40, 98, 207, 300	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	226	GLY	5.4
2	R	252	PRO	5.2
2	I	258	ASN	5.0
2	D	254	ALA	4.5
2	D	258	ASN	4.3
1	Z	372	PRO	4.3
1	Y	372	PRO	4.2
2	I	131	THR	4.1
2	G	224	PHE	4.1
2	I	183	ASN	4.0
2	F	172	ASN	3.9
2	Q	9	PHE	3.9
2	I	252	PRO	3.9
2	P	252	PRO	3.8
2	R	172	ASN	3.8
2	H	168	VAL	3.8
2	F	245	GLY	3.8
2	P	258	ASN	3.8
2	P	259	GLY	3.7
2	R	258	ASN	3.6
2	Q	160	ASP	3.6
2	Q	260	SER	3.5
2	R	131	THR	3.5
2	E	179	THR	3.5
2	R	253	ILE	3.5
2	I	244	TRP	3.5
2	H	242	THR	3.4
2	Q	246	ALA	3.4
2	Q	167	THR	3.4
2	R	249	ASP	3.4
2	P	230	SER	3.4
2	G	229	THR	3.2
2	E	253	ILE	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	Q	251	THR	3.2
2	Q	168	VAL	3.2
2	I	200	GLY	3.2
2	E	193	SER	3.1
2	H	249	ASP	3.1
2	E	168	VAL	3.1
2	P	253	ILE	3.1
2	E	165	THR	3.1
2	G	252	PRO	3.1
2	D	226	GLY	3.0
2	G	182	ASN	3.0
2	Q	206	THR	3.0
2	H	253	ILE	3.0
2	G	258	ASN	3.0
2	I	137	LYS	2.9
2	H	207	TRP	2.9
1	Z	303	PRO	2.9
2	Q	249	ASP	2.9
2	R	47	LEU	2.8
2	I	124	ASP	2.8
2	I	201	TRP	2.8
2	H	198	GLN	2.8
2	H	234	ASP	2.8
2	Q	230	SER	2.8
2	I	242	THR	2.8
2	I	101	ALA	2.8
2	G	164	GLN	2.8
2	P	223	HIS	2.8
2	H	208	VAL	2.8
2	H	193	SER	2.8
2	R	52	ASN	2.8
2	I	215	ALA	2.7
2	G	215	ALA	2.7
2	F	78	GLY	2.7
3	X	159	ILE	2.7
2	Q	195	SER	2.7
2	P	168	VAL	2.7
2	R	245	GLY	2.7
2	D	251	THR	2.7
2	E	167	THR	2.7
2	E	258	ASN	2.6
2	G	264	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	P	167	THR	2.6
2	P	192	GLY	2.6
2	G	168	VAL	2.6
2	R	256	ARG	2.6
2	P	257	GLY	2.6
2	H	252	PRO	2.6
2	E	209	ASP	2.6
2	B	246	ALA	2.6
2	H	246	ALA	2.6
1	Y	252	ALA	2.5
2	G	259	GLY	2.5
2	H	172	ASN	2.5
2	F	234	ASP	2.5
2	R	133	VAL	2.5
2	R	48	ASN	2.5
2	Q	171	GLY	2.5
2	F	135	SER	2.5
2	G	175	GLN	2.5
2	P	13	SER	2.5
2	G	169	GLU	2.5
2	R	254	ALA	2.5
2	G	184	ASP	2.5
2	J	228	ASP	2.5
2	R	229	THR	2.5
1	Z	158	ALA	2.5
2	F	246	ALA	2.5
1	1	372	PRO	2.5
2	H	260	SER	2.5
2	D	193	SER	2.4
2	F	249	ASP	2.4
2	Q	170	ALA	2.4
2	G	227	ARG	2.4
2	R	219	SER	2.4
2	F	230	SER	2.4
2	D	170	ALA	2.4
2	E	257	GLY	2.4
2	H	160	ASP	2.4
2	H	167	THR	2.4
2	H	53	VAL	2.4
2	G	195	SER	2.4
2	H	209	ASP	2.4
2	H	238	ASN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	31	THR	2.4
2	P	222	GLY	2.4
2	P	228	ASP	2.4
2	P	251	THR	2.4
2	G	253	ILE	2.4
2	H	218	GLN	2.4
2	Q	200	GLY	2.4
2	P	226	GLY	2.4
2	R	226	GLY	2.4
2	E	219	SER	2.4
2	H	204	SER	2.4
2	I	234	ASP	2.4
2	C	258	ASN	2.4
2	H	240	SER	2.3
2	R	230	SER	2.3
2	H	62	ALA	2.3
2	I	79	ASP	2.3
2	Q	222	GLY	2.3
2	I	84	ILE	2.3
2	H	184	ASP	2.3
2	D	222	GLY	2.3
2	F	101	ALA	2.3
2	H	257	GLY	2.3
2	G	163	VAL	2.3
2	D	175	GLN	2.3
2	P	200	GLY	2.3
2	H	215	ALA	2.3
2	F	79	ASP	2.3
2	F	251	THR	2.3
2	F	196	ASN	2.3
2	L	200	GLY	2.3
2	D	225	ALA	2.3
2	D	252	PRO	2.3
2	H	76	LEU	2.3
2	Q	257	GLY	2.3
1	1	320	THR	2.3
2	D	168	VAL	2.3
2	F	126	VAL	2.3
2	Q	159	ILE	2.3
2	I	198	GLN	2.2
2	F	82	ASN	2.2
2	Q	182	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	257	GLY	2.2
2	F	250	LYS	2.2
2	P	193	SER	2.2
2	F	125	ILE	2.2
2	F	259	GLY	2.2
2	R	223	HIS	2.2
2	D	255	THR	2.2
2	F	216	ALA	2.2
2	D	259	GLY	2.2
2	I	257	GLY	2.2
2	I	147	SER	2.2
1	1	300	HIS	2.2
1	Z	300	HIS	2.2
2	F	242	THR	2.2
2	F	258	ASN	2.2
2	G	230	SER	2.2
2	R	201	TRP	2.2
2	H	164	GLN	2.2
2	F	53	VAL	2.1
2	I	254	ALA	2.1
1	1	314	SER	2.1
2	M	48	ASN	2.1
2	Q	207	TRP	2.1
1	1	120	ASP	2.1
2	E	259	GLY	2.1
2	Q	31	THR	2.1
2	Q	253	ILE	2.1
2	H	79	ASP	2.1
2	M	100	SER	2.1
2	G	225	ALA	2.1
3	W	1	GLY	2.1
1	1	299	ASP	2.1
2	H	183	ASN	2.1
2	Q	248	ILE	2.1
1	1	305	GLU	2.1
2	R	171	GLY	2.1
2	P	31	THR	2.1
2	I	196	ASN	2.1
2	Q	209	ASP	2.1
2	G	247	ASN	2.1
2	P	215	ALA	2.1
2	P	175	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	R	255	THR	2.1
2	F	257	GLY	2.1
2	H	116	SER	2.0
2	H	165	THR	2.0
2	R	261	TYR	2.0
2	E	166	LEU	2.0
2	G	214	PRO	2.0
2	G	251	THR	2.0
2	H	251	THR	2.0
1	Y	251	LYS	2.0
2	E	200	GLY	2.0
2	I	202	ASN	2.0
2	R	234	ASP	2.0
2	I	223	HIS	2.0
2	R	250	LYS	2.0
2	H	171	GLY	2.0
1	Z	164	ASN	2.0
1	Y	164	ASN	2.0
2	G	223	HIS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	SR	V	1299	1/1	0.96	0.26	2.89	80,80,80,80	0
4	SR	W	1299	1/1	0.98	0.29	1.96	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	SR	T	1299	1/1	0.98	0.27	1.76	80,80,80,80	0
4	SR	X	1299	1/1	0.97	0.25	0.38	83,83,83,83	0
4	SR	S	1299	1/1	0.94	0.25	0.14	87,87,87,87	0
4	SR	U	1299	1/1	0.93	0.26	-	82,82,82,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.