



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:36 AM UTC

PDB ID : 5N8P / pdb_00005n8p
Title : S-layer protein RsaA from *C. crescentus*
Authors : Bharat, T.A.M.; Kureisaite-Ciziene, D.; Lowe, J.
Deposited on : 2017-02-24
Resolution : 2.70 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:

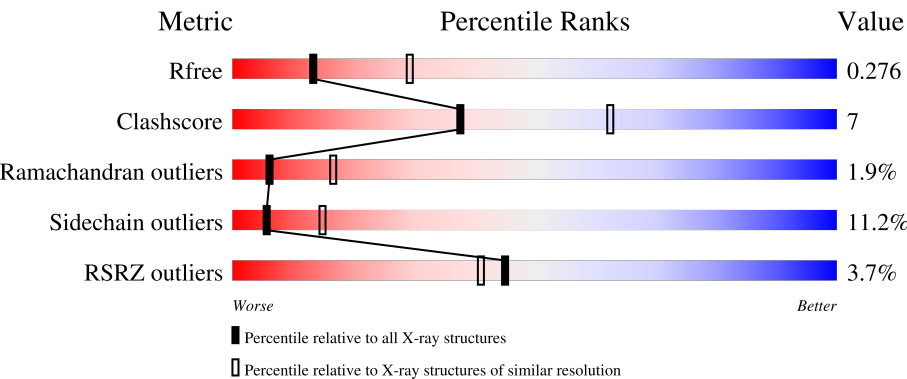
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	A	1026	2% 60% 13% • 24%
1	B	1026	3% 59% 14% • 24%
1	C	1026	3% 59% 14% • 24%
1	D	1026	2% 60% 13% • 24%
1	E	1026	3% 59% 14% • 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1026	4% 60% 14% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 31059 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 S-layer protein.

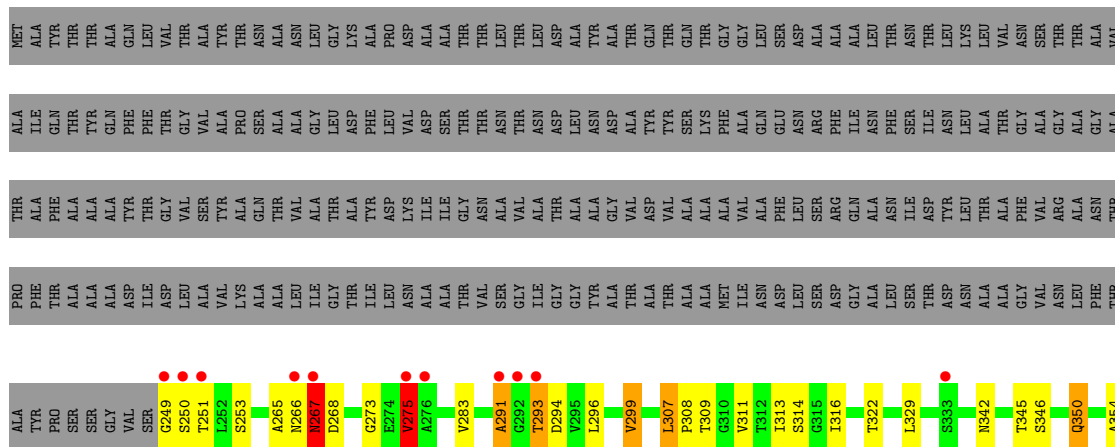
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	B	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	C	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	D	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	E	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			
1	F	778	Total	C	N	O	S	0	0	0
			5133	3124	862	1145	2			

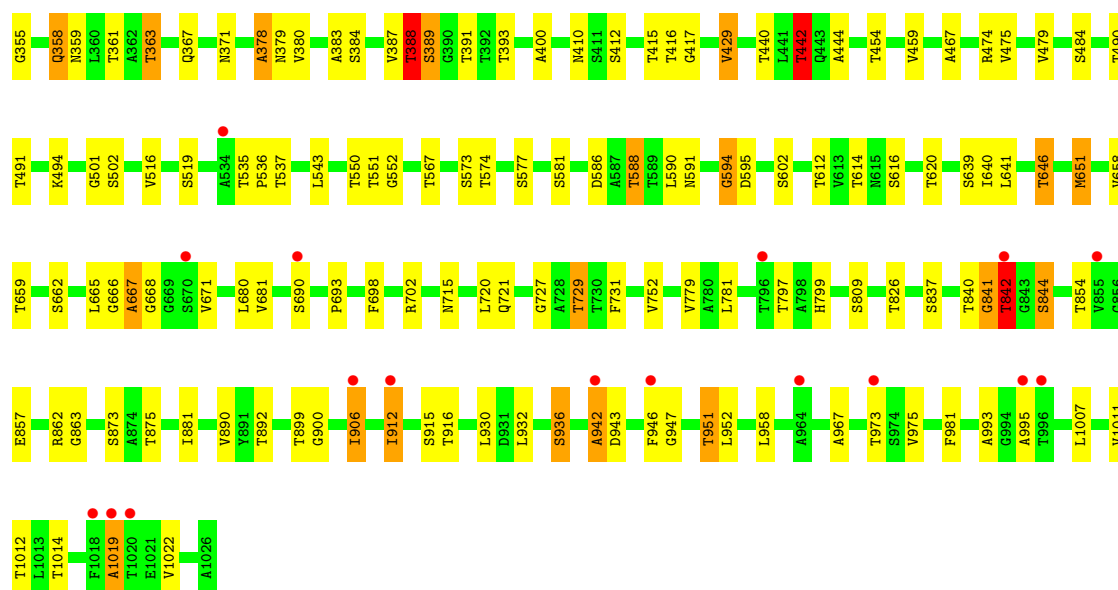
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	Ca	0	0
			19	19		
2	B	19	Total	Ca	0	0
			19	19		
2	C	19	Total	Ca	0	0
			19	19		
2	D	19	Total	Ca	0	0
			19	19		
2	E	19	Total	Ca	0	0
			19	19		
2	F	19	Total	Ca	0	0
			19	19		

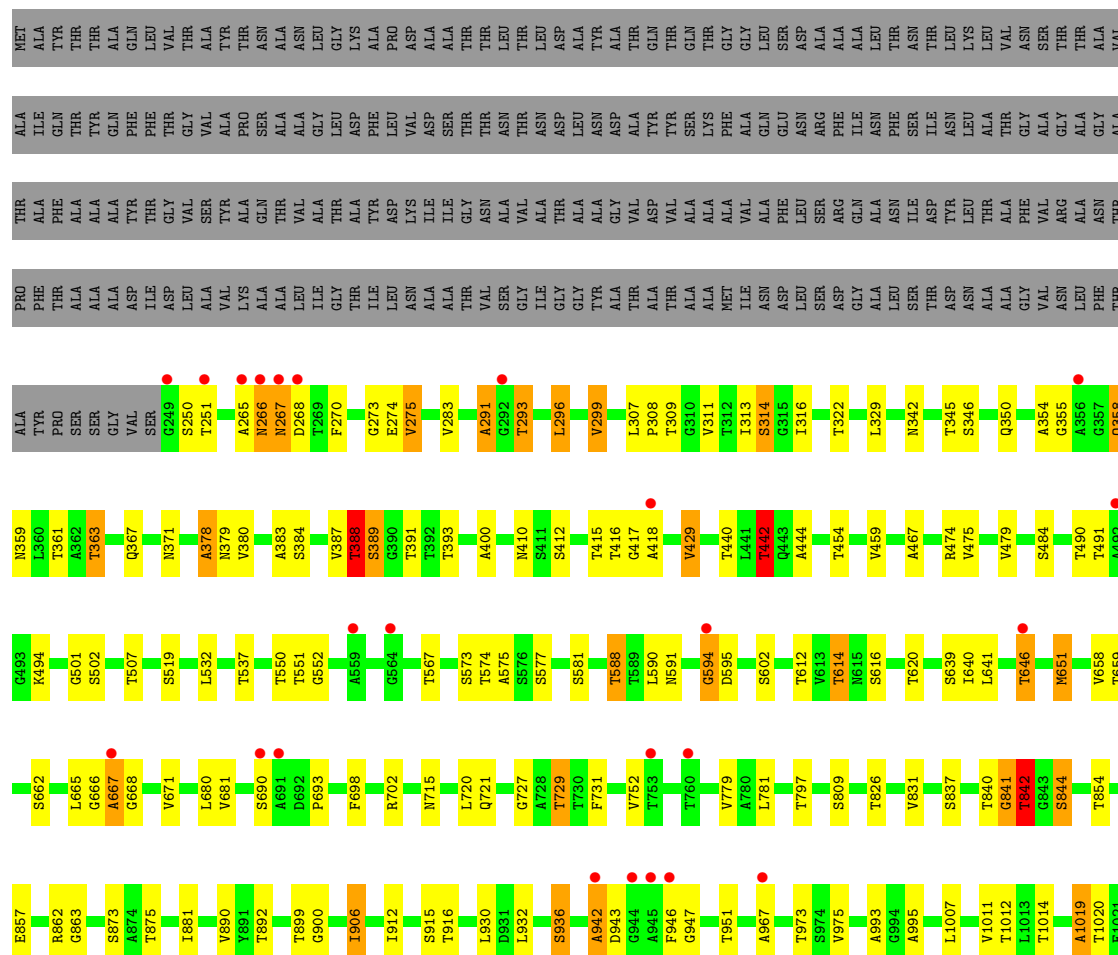
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	29	Total 29	O 29	0	0
3	C	24	Total 24	O 24	0	0
3	D	32	Total 32	O 32	0	0
3	E	16	Total 16	O 16	0	0
3	F	27	Total 27	O 27	0	0





• Molecule 1: S-layer protein



- Molecule 1: S-layer protein

D969	G970	S971	G972	T973	S974	V975	F981	A993	G994	A995	L1007	V1011	T1012	L1013	T1014	A1019	T1020	E1021	V1022	L1025	A1026
------	------	------	------	------	------	------	------	------	------	------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

- Molecule 1: S-layer protein

THR	ALA	ALA	PHE	ALA	ALA	ALA	ALA	ALA	TYR	THR	GLY	VAL	SER	TYR	ALA	GLN	THR	VAL	ALA	THR	ALA	TYR	ASP	LYS	ILE	ILE	GLY	ASN	VAL	VAL	ALA	ALA	ALA	THR	ALA	ALA	GLY	VAL	ASP	VAL	VAL	ALA	ALA	PHE	LEU	SER	SER	ARG	GLN	ALA	ASN	ILE	ASP	TYR	LEU	THR	ALA	PHE	VAL	ARG	ALA	ASN	THR
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

PRO	ALA	ALA	THR	ALA	ALA	ASP	ILE	ASP	LEU	ALA	VAL	LYS	ALA	ALA	LEU	GLY	THR	ILE	LEU	ASN	ALA	ALA	THR	VAL	SER	GLY	ILE	GLY	TYR	ALA	THR	ALA	ALA	MET	ILE	ASN	ASP	LEU	SER	THR	ASP	ASN	ALA	ALA	GLY	VAL	ASN	LEU	PHE	THR
																																					</													

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	215.88Å 74.96Å 221.66Å 90.00° 118.99° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	69.6 (50.00-2.70) 69.6 (50.00-2.70)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.258 , 0.276 0.258 , 0.276	Depositor DCC
R_{free} test set	6102 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 8.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.028 for -h-l,k,h 0.028 for l,k,-h-l 0.028 for h,-k,-h-l 0.026 for -h-l,-k,l 0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	31059	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.5499e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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:
CA

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	A	0.98	5/5166 (0.1%)	1.22	16/7112 (0.2%)
1	B	0.96	5/5166 (0.1%)	1.22	18/7112 (0.3%)
1	C	0.98	5/5166 (0.1%)	1.23	22/7112 (0.3%)
1	D	0.99	5/5166 (0.1%)	1.22	22/7112 (0.3%)
1	E	0.97	4/5166 (0.1%)	1.22	21/7112 (0.3%)
1	F	0.98	5/5166 (0.1%)	1.22	17/7112 (0.2%)
All	All	0.98	29/30996 (0.1%)	1.22	116/42672 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	842	THR	CA-CB	9.35	1.69	1.53
1	B	842	THR	CA-CB	8.80	1.68	1.53
1	A	842	THR	CA-CB	8.60	1.68	1.53
1	E	842	THR	CA-CB	8.43	1.67	1.53
1	C	842	THR	CA-CB	8.16	1.67	1.53
1	D	842	THR	CA-CB	8.08	1.67	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	842	THR	N-CA	6.54	1.54	1.46
1	A	842	THR	N-CA	6.32	1.54	1.46
1	E	841	GLY	N-CA	6.25	1.53	1.45
1	D	842	THR	N-CA	6.21	1.54	1.46
1	F	842	THR	N-CA	6.19	1.54	1.46
1	A	841	GLY	N-CA	5.89	1.53	1.45
1	E	1025	LEU	C-N	5.89	1.41	1.33
1	B	842	THR	N-CA	5.84	1.53	1.46
1	F	841	GLY	N-CA	5.82	1.53	1.45
1	D	841	GLY	N-CA	5.70	1.52	1.45
1	C	842	THR	N-CA	5.68	1.53	1.46
1	F	840	THR	CA-C	5.68	1.60	1.52
1	B	841	GLY	N-CA	5.65	1.52	1.45
1	C	840	THR	CA-C	5.64	1.60	1.52
1	F	484	SER	N-CA	5.47	1.52	1.46
1	C	841	GLY	N-CA	5.34	1.52	1.45
1	A	840	THR	CA-C	5.31	1.59	1.52
1	B	840	THR	CA-C	5.24	1.59	1.52
1	C	484	SER	N-CA	5.24	1.52	1.46
1	A	906	ILE	CA-CB	5.13	1.60	1.54
1	D	484	SER	N-CA	5.09	1.52	1.46
1	D	840	THR	CA-C	5.08	1.59	1.52
1	B	906	ILE	CA-CB	5.08	1.60	1.54

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	840	THR	N-CA-C	12.61	129.68	114.04
1	E	840	THR	N-CA-C	12.50	129.54	114.04
1	C	840	THR	N-CA-C	12.21	129.18	114.04
1	D	840	THR	N-CA-C	12.11	129.05	114.04
1	F	840	THR	N-CA-C	12.10	129.04	114.04
1	A	840	THR	N-CA-C	12.02	128.95	114.04
1	E	387	VAL	N-CA-C	10.62	120.40	110.74
1	C	387	VAL	N-CA-C	10.42	120.22	110.74
1	A	387	VAL	N-CA-C	10.14	119.97	110.74
1	F	387	VAL	N-CA-C	9.96	119.80	110.74
1	B	387	VAL	N-CA-C	9.91	119.76	110.74
1	D	387	VAL	N-CA-C	9.80	119.66	110.74
1	F	594	GLY	N-CA-C	7.56	120.75	111.45
1	E	594	GLY	N-CA-C	7.48	120.65	111.45
1	A	594	GLY	N-CA-C	7.36	120.51	111.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	594	GLY	N-CA-C	7.34	120.48	111.45
1	D	594	GLY	N-CA-C	7.31	120.45	111.45
1	B	594	GLY	N-CA-C	7.31	120.44	111.45
1	A	275	VAL	CB-CA-C	7.14	117.78	111.71
1	D	275	VAL	CB-CA-C	6.66	117.37	111.71
1	F	275	VAL	CB-CA-C	6.66	117.37	111.71
1	A	841	GLY	N-CA-C	6.64	121.98	112.82
1	B	841	GLY	N-CA-C	6.52	121.82	112.82
1	D	639	SER	N-CA-C	6.42	118.53	107.93
1	B	275	VAL	CB-CA-C	6.39	117.14	111.71
1	E	906	ILE	CB-CA-C	6.27	119.67	110.77
1	E	841	GLY	N-CA-C	6.19	121.36	112.82
1	F	906	ILE	CB-CA-C	6.17	119.53	110.77
1	C	275	VAL	CB-CA-C	6.09	116.89	111.71
1	C	841	GLY	N-CA-C	6.09	121.23	112.82
1	C	906	ILE	CB-CA-C	6.04	119.35	110.77
1	E	291	ALA	N-CA-C	6.03	117.82	110.41
1	B	639	SER	N-CA-C	6.02	117.86	107.93
1	D	906	ILE	CB-CA-C	5.99	119.28	110.77
1	A	906	ILE	CB-CA-C	5.98	119.26	110.77
1	F	900	GLY	N-CA-C	-5.94	99.72	111.31
1	C	639	SER	N-CA-C	5.92	117.69	107.93
1	F	639	SER	N-CA-C	5.91	117.68	107.93
1	A	900	GLY	N-CA-C	-5.91	99.79	111.31
1	C	900	GLY	N-CA-C	-5.90	99.80	111.31
1	F	841	GLY	N-CA-C	5.90	120.96	112.82
1	D	841	GLY	N-CA-C	5.90	120.96	112.82
1	B	906	ILE	CB-CA-C	5.89	119.13	110.77
1	F	291	ALA	N-CA-C	5.88	117.64	110.41
1	D	291	ALA	N-CA-C	5.87	117.63	110.41
1	A	291	ALA	N-CA-C	5.85	117.60	110.41
1	A	639	SER	N-CA-C	5.78	117.55	107.49
1	E	900	GLY	N-CA-C	-5.76	100.08	111.31
1	C	389	SER	N-CA-C	5.76	119.12	111.75
1	E	275	VAL	N-CA-CB	5.67	117.18	111.57
1	E	389	SER	N-CA-C	5.66	118.99	111.75
1	D	389	SER	N-CA-C	5.62	118.94	111.75
1	E	275	VAL	CB-CA-C	5.57	116.45	111.71
1	B	442	THR	CB-CA-C	5.55	118.92	109.75
1	A	388	THR	N-CA-C	5.53	116.18	108.00
1	B	307	LEU	CA-C-N	-5.53	114.89	120.31
1	B	307	LEU	C-N-CA	-5.53	114.89	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	639	SER	N-CA-C	5.52	117.04	107.93
1	D	900	GLY	N-CA-C	-5.51	100.56	111.31
1	E	307	LEU	CA-C-N	-5.51	114.91	120.31
1	E	307	LEU	C-N-CA	-5.51	114.91	120.31
1	E	890	VAL	N-CA-C	5.49	115.85	108.17
1	D	442	THR	CB-CA-C	5.48	118.80	109.75
1	F	389	SER	N-CA-C	5.46	118.75	111.75
1	C	275	VAL	CA-C-N	-5.41	114.10	123.25
1	C	275	VAL	C-N-CA	-5.41	114.10	123.25
1	A	389	SER	N-CA-C	5.41	118.68	111.75
1	A	890	VAL	N-CA-C	5.40	115.73	108.17
1	D	307	LEU	CA-C-N	-5.39	115.03	120.31
1	D	307	LEU	C-N-CA	-5.39	115.03	120.31
1	E	442	THR	CB-CA-C	5.37	118.61	109.75
1	C	616	SER	N-CA-C	5.37	116.81	111.07
1	A	442	THR	CB-CA-C	5.34	118.57	109.75
1	F	442	THR	CB-CA-C	5.34	118.56	109.75
1	C	442	THR	CB-CA-C	5.33	118.54	109.75
1	B	900	GLY	N-CA-C	-5.32	100.94	111.31
1	D	388	THR	N-CA-C	5.31	115.86	108.00
1	B	291	ALA	N-CA-C	5.29	116.92	110.41
1	A	646	THR	N-CA-C	-5.29	106.84	113.72
1	B	389	SER	N-CA-C	5.29	118.51	111.75
1	C	842	THR	N-CA-CB	5.27	119.40	110.49
1	E	275	VAL	CA-C-N	-5.25	114.37	123.25
1	E	275	VAL	C-N-CA	-5.25	114.37	123.25
1	B	388	THR	N-CA-C	5.25	115.76	108.00
1	D	890	VAL	N-CA-C	5.24	115.51	108.17
1	C	890	VAL	N-CA-C	5.23	115.50	108.17
1	B	294	ASP	N-CA-C	5.23	117.76	109.24
1	C	307	LEU	CA-C-N	-5.23	115.19	120.31
1	C	307	LEU	C-N-CA	-5.23	115.19	120.31
1	C	388	THR	N-CA-C	5.23	115.74	108.00
1	D	831	VAL	N-CA-C	5.23	115.13	108.12
1	F	616	SER	N-CA-C	5.21	116.65	111.07
1	E	616	SER	N-CA-C	5.21	116.64	111.07
1	C	294	ASP	N-CA-C	5.20	117.71	109.24
1	B	616	SER	N-CA-C	5.17	116.60	111.07
1	B	646	THR	N-CA-C	-5.17	107.00	113.72
1	E	388	THR	N-CA-C	5.17	115.65	108.00
1	F	388	THR	N-CA-C	5.17	115.65	108.00
1	E	253	SER	N-CA-C	5.16	117.14	108.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	890	VAL	N-CA-C	5.13	115.35	108.17
1	F	890	VAL	N-CA-C	5.13	115.35	108.17
1	D	614	THR	N-CA-C	-5.13	105.79	113.89
1	A	842	THR	N-CA-CB	5.12	119.14	110.49
1	C	291	ALA	N-CA-C	5.12	116.71	110.41
1	A	616	SER	N-CA-C	5.12	116.55	111.07
1	D	275	VAL	CA-C-N	-5.11	114.61	123.25
1	D	275	VAL	C-N-CA	-5.11	114.61	123.25
1	C	646	THR	N-CA-C	-5.11	107.08	113.72
1	D	616	SER	N-CA-C	5.09	116.52	111.07
1	D	646	THR	N-CA-C	-5.07	107.12	113.72
1	D	842	THR	N-CA-CB	5.06	119.05	110.49
1	F	614	THR	N-CA-C	-5.05	105.91	113.89
1	E	294	ASP	N-CA-C	5.03	117.43	109.24
1	F	842	THR	CA-CB-CG2	5.03	119.05	110.50
1	F	842	THR	N-CA-CB	5.03	118.98	110.49
1	C	253	SER	N-CA-C	5.02	116.91	108.73

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	594	GLY	Peptide
1	B	594	GLY	Peptide
1	C	594	GLY	Peptide
1	D	594	GLY	Peptide
1	E	594	GLY	Peptide
1	F	594	GLY	Peptide

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	A	5133	0	5071	65	0
1	B	5133	0	5071	75	0
1	C	5133	0	5071	71	8
1	D	5133	0	5071	73	7

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	5133	0	5071	75	0
1	F	5133	0	5072	72	1
2	A	19	0	0	0	0
2	B	19	0	0	1	0
2	C	19	0	0	1	0
2	D	19	0	0	0	0
2	E	19	0	0	0	0
2	F	19	0	0	4	0
3	A	19	0	0	1	0
3	B	29	0	0	3	0
3	C	24	0	0	3	0
3	D	32	0	0	5	0
3	E	16	0	0	9	0
3	F	27	0	0	10	0
All	All	31059	0	30427	430	8

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (430) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9002:CA:CA	3:C:9103:HOH:O	1.22	1.11
2:F:9007:CA:CA	3:F:9103:HOH:O	1.30	1.07
1:D:265:ALA:HA	1:D:291:ALA:H	1.22	1.04
1:F:265:ALA:HA	1:F:291:ALA:H	1.22	1.02
1:E:265:ALA:HA	1:E:291:ALA:H	1.22	1.01
1:F:864:GLY:O	3:F:9102:HOH:O	1.78	1.00
1:A:265:ALA:HA	1:A:291:ALA:H	1.22	0.99
1:B:265:ALA:HA	1:B:291:ALA:H	1.21	0.98
1:C:265:ALA:HA	1:C:291:ALA:H	1.22	0.98
1:D:274:GLU:O	3:D:9101:HOH:O	1.82	0.98
2:F:9003:CA:CA	3:F:9101:HOH:O	1.41	0.95
1:F:282:THR:OG1	3:F:9101:HOH:O	1.67	0.90
2:F:9011:CA:CA	3:F:9102:HOH:O	1.51	0.87
1:F:656:ASP:OD2	3:F:9103:HOH:O	1.93	0.86
1:D:442:THR:HB	1:D:475:VAL:HB	1.60	0.83
1:C:442:THR:HB	1:C:475:VAL:HB	1.60	0.83
1:F:442:THR:HB	1:F:475:VAL:HB	1.60	0.82
1:B:442:THR:HB	1:B:475:VAL:HB	1.59	0.82
1:E:442:THR:HB	1:E:475:VAL:HB	1.60	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:THR:HB	1:A:475:VAL:HB	1.61	0.80
2:B:9002:CA:CA	3:B:9103:HOH:O	1.62	0.76
1:B:255:THR:O	3:B:9101:HOH:O	2.04	0.75
1:F:652:GLY:O	3:F:9103:HOH:O	2.06	0.73
1:B:342:ASN:HD22	1:B:361:THR:HB	1.54	0.72
1:D:342:ASN:HD22	1:D:361:THR:HB	1.55	0.71
1:F:342:ASN:HD22	1:F:361:THR:HB	1.55	0.71
1:F:884:ALA:O	3:F:9102:HOH:O	2.08	0.71
1:E:342:ASN:HD22	1:E:361:THR:HB	1.56	0.70
1:A:342:ASN:HD22	1:A:361:THR:HB	1.55	0.70
1:A:265:ALA:HA	1:A:291:ALA:N	2.04	0.70
1:E:725:THR:CG2	3:E:9101:HOH:O	2.38	0.70
1:F:640:ILE:HG12	1:F:651:MET:HE1	1.74	0.69
1:B:265:ALA:HA	1:B:291:ALA:N	2.04	0.69
1:C:342:ASN:HD22	1:C:361:THR:HB	1.56	0.69
1:D:314:SER:HB3	3:D:9110:HOH:O	1.92	0.69
1:E:265:ALA:HA	1:E:291:ALA:N	2.04	0.68
1:D:947:GLY:O	1:D:1014:THR:HA	1.94	0.68
1:F:702:ARG:HB2	1:F:721:GLN:HB2	1.76	0.68
1:F:947:GLY:O	1:F:1014:THR:HA	1.94	0.67
1:A:947:GLY:O	1:A:1014:THR:HA	1.94	0.67
1:C:947:GLY:O	1:C:1014:THR:HA	1.94	0.67
1:C:265:ALA:HA	1:C:291:ALA:N	2.04	0.67
1:F:265:ALA:HA	1:F:291:ALA:N	2.04	0.67
1:E:947:GLY:O	1:E:1014:THR:HA	1.94	0.67
1:E:640:ILE:HG12	1:E:651:MET:HE1	1.75	0.67
1:B:947:GLY:O	1:B:1014:THR:HA	1.94	0.67
1:A:640:ILE:HG12	1:A:651:MET:HE1	1.77	0.66
1:A:702:ARG:HB2	1:A:721:GLN:HB2	1.75	0.66
1:E:702:ARG:HB2	1:E:721:GLN:HB2	1.77	0.66
1:B:640:ILE:HG12	1:B:651:MET:HE1	1.77	0.66
1:C:640:ILE:HG12	1:C:651:MET:HE1	1.77	0.66
1:D:640:ILE:HG12	1:D:651:MET:HE1	1.76	0.66
1:B:702:ARG:HB2	1:B:721:GLN:HB2	1.77	0.66
1:D:702:ARG:HB2	1:D:721:GLN:HB2	1.77	0.66
1:D:265:ALA:HA	1:D:291:ALA:N	2.04	0.65
1:B:841:GLY:H	1:B:844:SER:HG	1.44	0.65
1:C:702:ARG:HB2	1:C:721:GLN:HB2	1.77	0.65
1:C:586:ASP:OD2	3:C:9101:HOH:O	2.15	0.64
1:E:725:THR:HG23	3:E:9101:HOH:O	1.95	0.64
1:C:841:GLY:H	1:C:844:SER:HG	1.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:841:GLY:H	1:E:844:SER:HG	1.46	0.63
1:E:703:VAL:O	3:E:9101:HOH:O	2.16	0.62
1:D:842:THR:HG21	3:D:9102:HOH:O	1.99	0.62
1:D:842:THR:CG2	3:D:9102:HOH:O	2.47	0.61
1:E:704:ALA:HA	3:E:9101:HOH:O	2.00	0.61
1:D:265:ALA:CA	1:D:291:ALA:H	2.08	0.60
1:D:532:LEU:HD13	3:D:9105:HOH:O	2.01	0.60
1:A:841:GLY:N	1:A:844:SER:OG	2.33	0.60
1:B:841:GLY:N	1:B:844:SER:OG	2.33	0.59
1:D:841:GLY:N	1:D:844:SER:OG	2.33	0.59
1:E:265:ALA:CA	1:E:291:ALA:H	2.08	0.58
1:C:265:ALA:CA	1:C:291:ALA:H	2.08	0.58
2:F:9019:CA:CA	3:F:9107:HOH:O	1.78	0.58
1:D:416:THR:O	1:D:416:THR:HG22	2.04	0.58
1:E:410:ASN:OD1	1:E:412:SER:HB3	2.04	0.58
1:A:359:ASN:ND2	1:A:379:ASN:H	2.02	0.58
1:B:440:THR:OG1	1:B:467:ALA:HB2	2.04	0.57
1:F:501:GLY:HA2	1:F:519:SER:HB3	1.86	0.57
1:F:912:ILE:HD12	1:F:912:ILE:H	1.69	0.57
1:B:501:GLY:HA2	1:B:519:SER:HB3	1.86	0.57
1:C:410:ASN:OD1	1:C:412:SER:HB3	2.04	0.57
1:D:410:ASN:OD1	1:D:412:SER:HB3	2.05	0.57
1:A:265:ALA:CA	1:A:291:ALA:H	2.08	0.57
1:A:440:THR:OG1	1:A:467:ALA:HB2	2.04	0.57
1:B:416:THR:HG22	1:B:416:THR:O	2.04	0.57
1:E:416:THR:HG22	1:E:416:THR:O	2.05	0.57
1:C:841:GLY:N	1:C:844:SER:OG	2.33	0.57
1:A:410:ASN:OD1	1:A:412:SER:HB3	2.05	0.57
1:A:1019:ALA:HB3	1:A:1022:VAL:HB	1.87	0.57
1:B:410:ASN:OD1	1:B:412:SER:HB3	2.04	0.57
1:C:501:GLY:HA2	1:C:519:SER:HB3	1.87	0.57
1:E:359:ASN:ND2	1:E:379:ASN:H	2.02	0.57
1:F:410:ASN:OD1	1:F:412:SER:HB3	2.04	0.57
1:C:440:THR:OG1	1:C:467:ALA:HB2	2.05	0.57
1:C:799:HIS:HB3	3:C:9123:HOH:O	2.04	0.57
1:F:359:ASN:ND2	1:F:379:ASN:H	2.03	0.57
1:F:440:THR:OG1	1:F:467:ALA:HB2	2.05	0.57
1:D:313:ILE:HG23	1:D:316:ILE:HD12	1.86	0.56
1:D:359:ASN:ND2	1:D:379:ASN:H	2.03	0.56
1:C:359:ASN:ND2	1:C:379:ASN:H	2.03	0.56
1:D:912:ILE:HD12	1:D:912:ILE:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1019:ALA:HB3	1:E:1022:VAL:HB	1.88	0.56
1:A:359:ASN:HD22	1:A:379:ASN:H	1.54	0.56
1:A:416:THR:O	1:A:416:THR:HG22	2.05	0.56
1:C:313:ILE:HG23	1:C:316:ILE:HD12	1.88	0.56
1:C:416:THR:HG22	1:C:416:THR:O	2.05	0.56
1:D:501:GLY:HA2	1:D:519:SER:HB3	1.88	0.56
1:A:501:GLY:HA2	1:A:519:SER:HB3	1.87	0.56
1:E:440:THR:OG1	1:E:467:ALA:HB2	2.05	0.56
1:F:1019:ALA:HB3	1:F:1022:VAL:HB	1.87	0.56
1:B:313:ILE:HG23	1:B:316:ILE:HD12	1.88	0.56
1:C:912:ILE:H	1:C:912:ILE:HD12	1.70	0.55
1:D:440:THR:OG1	1:D:467:ALA:HB2	2.06	0.55
1:B:359:ASN:ND2	1:B:379:ASN:H	2.03	0.55
1:C:1019:ALA:HB3	1:C:1022:VAL:HB	1.87	0.55
1:A:841:GLY:H	1:A:844:SER:HG	1.53	0.55
1:E:501:GLY:HA2	1:E:519:SER:HB3	1.87	0.55
1:A:313:ILE:HG23	1:A:316:ILE:HD12	1.89	0.55
1:E:359:ASN:HD22	1:E:379:ASN:H	1.54	0.55
1:E:841:GLY:N	1:E:844:SER:OG	2.33	0.55
1:F:416:THR:O	1:F:416:THR:HG22	2.05	0.55
1:C:359:ASN:HD22	1:C:379:ASN:H	1.55	0.54
1:D:1019:ALA:HB3	1:D:1022:VAL:HB	1.89	0.54
1:B:265:ALA:CA	1:B:291:ALA:H	2.08	0.54
1:F:313:ILE:HG23	1:F:316:ILE:HD12	1.90	0.54
1:C:715:ASN:ND2	1:D:693:PRO:HB3	2.23	0.54
1:B:1019:ALA:HB3	1:B:1022:VAL:HB	1.88	0.54
1:E:912:ILE:H	1:E:912:ILE:HD12	1.71	0.53
1:C:693:PRO:HB3	1:D:715:ASN:ND2	2.23	0.53
1:E:354:ALA:HB1	1:E:358:GLN:HE21	1.74	0.53
1:E:313:ILE:HG23	1:E:316:ILE:HD12	1.89	0.53
1:A:354:ALA:HB1	1:A:358:GLN:HE21	1.74	0.53
1:C:265:ALA:C	1:C:291:ALA:HB3	2.34	0.53
1:D:354:ALA:HB1	1:D:358:GLN:HE21	1.74	0.53
1:E:405:SER:HB3	3:E:9108:HOH:O	2.08	0.53
1:A:912:ILE:HD12	1:A:912:ILE:H	1.73	0.52
1:D:273:GLY:HA2	1:D:299:VAL:HG23	1.91	0.52
1:A:754:LEU:HD23	3:A:9115:HOH:O	2.09	0.52
1:B:359:ASN:HD22	1:B:379:ASN:H	1.55	0.52
1:B:837:SER:HA	1:B:863:GLY:O	2.10	0.52
1:C:273:GLY:HA2	1:C:299:VAL:HG23	1.92	0.52
1:C:354:ALA:HB1	1:C:358:GLN:HE21	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:ASN:HD22	1:D:379:ASN:H	1.56	0.52
1:F:265:ALA:C	1:F:291:ALA:HB3	2.35	0.52
1:F:354:ALA:HB1	1:F:358:GLN:HE21	1.75	0.52
1:F:841:GLY:N	1:F:844:SER:OG	2.33	0.52
1:B:354:ALA:HB1	1:B:358:GLN:HE21	1.75	0.51
1:F:273:GLY:HA2	1:F:299:VAL:HG23	1.90	0.51
1:A:265:ALA:C	1:A:291:ALA:HB3	2.35	0.51
1:C:367:GLN:NE2	1:C:384:SER:HB3	2.25	0.51
1:F:359:ASN:HD22	1:F:379:ASN:H	1.56	0.51
1:B:367:GLN:NE2	1:B:384:SER:HB3	2.26	0.51
1:C:416:THR:HB	1:C:444:ALA:HB2	1.92	0.51
1:F:930:LEU:HG	1:F:932:LEU:HD21	1.93	0.51
1:B:912:ILE:HD12	1:B:912:ILE:H	1.75	0.51
1:D:837:SER:HA	1:D:863:GLY:O	2.11	0.51
1:B:273:GLY:HA2	1:B:299:VAL:HG23	1.91	0.51
1:D:265:ALA:C	1:D:291:ALA:HB3	2.35	0.51
1:E:265:ALA:C	1:E:291:ALA:HB3	2.35	0.51
1:A:416:THR:HB	1:A:444:ALA:HB2	1.93	0.51
1:A:837:SER:HA	1:A:863:GLY:O	2.11	0.51
1:B:265:ALA:C	1:B:291:ALA:HB3	2.36	0.51
1:E:720:LEU:HD13	1:E:731:PHE:CD1	2.46	0.51
1:E:837:SER:HA	1:E:863:GLY:O	2.11	0.51
1:A:273:GLY:HA2	1:A:299:VAL:HG23	1.91	0.51
1:A:930:LEU:HG	1:A:932:LEU:HD21	1.93	0.51
1:C:363:THR:HG23	1:C:383:ALA:HB3	1.92	0.51
1:C:837:SER:HA	1:C:863:GLY:O	2.11	0.51
1:A:367:GLN:NE2	1:A:384:SER:HB3	2.25	0.51
1:B:930:LEU:HG	1:B:932:LEU:HD21	1.91	0.50
1:E:930:LEU:HG	1:E:932:LEU:HD21	1.93	0.50
1:D:355:GLY:H	1:D:358:GLN:NE2	2.09	0.50
1:E:273:GLY:HA2	1:E:299:VAL:HG23	1.93	0.50
1:E:367:GLN:NE2	1:E:384:SER:HB3	2.26	0.50
1:B:435:ASN:O	3:B:9102:HOH:O	2.19	0.50
1:F:416:THR:HB	1:F:444:ALA:HB2	1.94	0.50
1:D:367:GLN:NE2	1:D:384:SER:HB3	2.27	0.50
1:F:942:ALA:O	1:F:943:ASP:CB	2.60	0.50
1:E:550:THR:HG22	1:E:552:GLY:H	1.77	0.50
1:B:720:LEU:HD13	1:B:731:PHE:CD1	2.47	0.50
1:F:837:SER:HA	1:F:863:GLY:O	2.11	0.50
1:A:415:THR:HB	1:A:442:THR:O	2.12	0.49
1:C:930:LEU:HG	1:C:932:LEU:HD21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:673:GLY:O	3:F:9103:HOH:O	2.20	0.49
1:B:388:THR:OG1	1:B:389:SER:N	2.46	0.49
1:E:388:THR:OG1	1:E:389:SER:N	2.46	0.49
1:F:388:THR:OG1	1:F:389:SER:N	2.45	0.49
1:B:363:THR:HG23	1:B:383:ALA:HB3	1.94	0.49
1:D:308:PRO:HD2	1:D:311:VAL:HG21	1.95	0.49
1:D:942:ALA:O	1:D:943:ASP:CB	2.59	0.49
1:E:942:ALA:O	1:E:943:ASP:CB	2.60	0.49
1:F:355:GLY:H	1:F:358:GLN:NE2	2.10	0.49
1:A:550:THR:HG22	1:A:552:GLY:H	1.77	0.49
1:B:416:THR:HB	1:B:444:ALA:HB2	1.94	0.49
1:E:371:ASN:ND2	1:E:391:THR:H	2.10	0.49
1:D:371:ASN:ND2	1:D:391:THR:H	2.10	0.49
1:D:720:LEU:HD13	1:D:731:PHE:CD1	2.47	0.49
1:A:942:ALA:O	1:A:943:ASP:CB	2.60	0.49
1:F:265:ALA:CA	1:F:291:ALA:H	2.08	0.49
1:F:363:THR:HG23	1:F:383:ALA:HB3	1.94	0.49
1:F:367:GLN:NE2	1:F:384:SER:HB3	2.26	0.49
1:C:942:ALA:O	1:C:943:ASP:CB	2.60	0.49
1:D:930:LEU:HG	1:D:932:LEU:HD21	1.93	0.49
1:A:371:ASN:ND2	1:A:391:THR:H	2.11	0.49
1:C:666:GLY:O	1:C:667:ALA:C	2.56	0.49
1:D:416:THR:HB	1:D:444:ALA:HB2	1.94	0.49
1:D:641:LEU:HG	1:D:659:THR:HB	1.95	0.49
1:F:720:LEU:HD13	1:F:731:PHE:CD1	2.48	0.49
1:F:666:GLY:O	1:F:667:ALA:C	2.56	0.49
1:B:415:THR:HB	1:B:442:THR:O	2.13	0.48
1:B:550:THR:HG22	1:B:552:GLY:H	1.78	0.48
1:E:416:THR:HB	1:E:444:ALA:HB2	1.93	0.48
1:F:415:THR:HB	1:F:442:THR:O	2.13	0.48
1:B:355:GLY:H	1:B:358:GLN:NE2	2.10	0.48
1:B:752:VAL:HB	1:B:781:LEU:HD23	1.95	0.48
1:C:715:ASN:HD21	1:D:693:PRO:HB3	1.78	0.48
1:C:720:LEU:HD13	1:C:731:PHE:CD1	2.48	0.48
1:A:363:THR:HG23	1:A:383:ALA:HB3	1.94	0.48
1:A:388:THR:OG1	1:A:389:SER:N	2.46	0.48
1:A:720:LEU:HD13	1:A:731:PHE:CD1	2.48	0.48
1:B:942:ALA:O	1:B:943:ASP:CB	2.60	0.48
1:D:388:THR:OG1	1:D:389:SER:N	2.46	0.48
1:C:388:THR:OG1	1:C:389:SER:N	2.46	0.48
1:D:550:THR:HG22	1:D:552:GLY:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:355:GLY:H	1:E:358:GLN:NE2	2.10	0.48
1:A:355:GLY:H	1:A:358:GLN:NE2	2.11	0.48
1:C:415:THR:HB	1:C:442:THR:O	2.13	0.48
1:C:550:THR:HG22	1:C:552:GLY:H	1.77	0.48
1:B:371:ASN:ND2	1:B:391:THR:H	2.11	0.48
1:E:363:THR:HG23	1:E:383:ALA:HB3	1.95	0.48
1:F:371:ASN:ND2	1:F:391:THR:H	2.11	0.48
1:C:355:GLY:H	1:C:358:GLN:NE2	2.11	0.48
1:A:666:GLY:O	1:A:667:ALA:C	2.56	0.48
1:C:371:ASN:ND2	1:C:391:THR:H	2.11	0.48
1:D:415:THR:HB	1:D:442:THR:O	2.13	0.48
1:E:666:GLY:O	1:E:667:ALA:C	2.56	0.48
1:E:752:VAL:HB	1:E:781:LEU:HD23	1.95	0.48
1:D:666:GLY:O	1:D:667:ALA:C	2.56	0.47
1:C:752:VAL:HB	1:C:781:LEU:HD23	1.96	0.47
1:E:415:THR:HB	1:E:442:THR:O	2.14	0.47
1:E:756:ASN:HB2	1:F:693:PRO:HD2	1.96	0.47
1:B:666:GLY:O	1:B:667:ALA:C	2.56	0.47
1:D:752:VAL:HB	1:D:781:LEU:HD23	1.96	0.47
1:F:641:LEU:HG	1:F:659:THR:HB	1.96	0.47
1:C:693:PRO:HB3	1:D:715:ASN:HD21	1.78	0.47
1:F:345:THR:HG22	1:F:346:SER:N	2.30	0.47
1:F:550:THR:HG22	1:F:552:GLY:H	1.78	0.47
1:A:345:THR:HG22	1:A:346:SER:N	2.30	0.47
1:A:752:VAL:HB	1:A:781:LEU:HD23	1.96	0.47
1:C:345:THR:HG22	1:C:346:SER:N	2.30	0.46
1:C:641:LEU:HG	1:C:659:THR:HB	1.97	0.46
1:E:345:THR:HG22	1:E:346:SER:N	2.31	0.46
1:F:752:VAL:HB	1:F:781:LEU:HD23	1.96	0.46
1:F:367:GLN:HE21	1:F:384:SER:HB3	1.79	0.46
1:B:345:THR:HG22	1:B:346:SER:N	2.31	0.46
1:D:345:THR:HG22	1:D:346:SER:N	2.30	0.46
1:B:641:LEU:HG	1:B:659:THR:HB	1.97	0.46
1:E:854:THR:HB	1:E:857:GLU:CG	2.46	0.46
1:B:350:GLN:HE21	1:B:350:GLN:HB2	1.57	0.46
1:B:573:SER:HA	1:B:595:ASP:HB3	1.98	0.46
1:C:308:PRO:HD2	1:C:311:VAL:HG21	1.98	0.46
1:C:535:THR:HA	1:C:536:PRO:HD3	1.82	0.46
1:D:854:THR:HB	1:D:857:GLU:CG	2.46	0.46
1:C:267:ASN:HA	1:C:293:THR:OG1	2.16	0.45
1:D:250:SER:H	1:D:268:ASP:HB3	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:936:SER:O	1:D:936:SER:OG	2.30	0.45
1:A:573:SER:HA	1:A:595:ASP:HB3	1.98	0.45
1:A:350:GLN:HE21	1:A:350:GLN:HB2	1.56	0.45
1:C:854:THR:HB	1:C:857:GLU:CG	2.46	0.45
1:E:267:ASN:HA	1:E:293:THR:OG1	2.16	0.45
1:F:854:THR:HB	1:F:857:GLU:CG	2.47	0.45
1:D:363:THR:HG23	1:D:383:ALA:HB3	1.99	0.45
1:A:267:ASN:HA	1:A:293:THR:OG1	2.16	0.45
1:C:573:SER:HA	1:C:595:ASP:HB3	1.99	0.45
1:B:267:ASN:HA	1:B:293:THR:OG1	2.16	0.45
1:D:841:GLY:O	1:D:842:THR:C	2.60	0.45
1:E:641:LEU:HG	1:E:659:THR:HB	1.99	0.45
1:F:267:ASN:HA	1:F:293:THR:OG1	2.16	0.45
1:A:854:THR:HB	1:A:857:GLU:CG	2.46	0.45
1:E:573:SER:HA	1:E:595:ASP:HB3	1.99	0.45
1:A:308:PRO:HD2	1:A:311:VAL:HG21	1.99	0.44
1:C:250:SER:H	1:C:268:ASP:HB3	1.82	0.44
1:C:841:GLY:O	1:C:842:THR:C	2.60	0.44
1:E:378:ALA:O	1:E:400:ALA:HB1	2.18	0.44
1:E:725:THR:HG22	3:E:9101:HOH:O	2.09	0.44
1:D:267:ASN:HA	1:D:293:THR:OG1	2.17	0.44
1:E:429:VAL:HG22	1:E:459:VAL:HG13	1.99	0.44
1:B:854:THR:HB	1:B:857:GLU:CG	2.46	0.44
1:E:529:ARG:NH2	3:E:9103:HOH:O	2.51	0.44
1:A:841:GLY:O	1:A:842:THR:C	2.60	0.44
1:B:367:GLN:HE21	1:B:384:SER:HB3	1.82	0.44
1:F:573:SER:HA	1:F:595:ASP:HB3	1.99	0.44
1:E:308:PRO:HD2	1:E:311:VAL:HG21	2.00	0.44
1:E:841:GLY:O	1:E:842:THR:C	2.60	0.44
1:A:378:ALA:O	1:A:400:ALA:HB1	2.18	0.44
1:C:367:GLN:HE21	1:C:384:SER:HB3	1.83	0.44
1:F:308:PRO:HD2	1:F:311:VAL:HG21	2.00	0.44
1:B:841:GLY:O	1:B:842:THR:C	2.60	0.44
1:C:378:ALA:O	1:C:400:ALA:HB1	2.18	0.44
1:C:429:VAL:HG22	1:C:459:VAL:HG13	1.99	0.43
1:C:581:SER:HA	1:C:602:SER:O	2.19	0.43
1:D:378:ALA:O	1:D:400:ALA:HB1	2.17	0.43
1:F:342:ASN:ND2	1:F:361:THR:HB	2.29	0.43
1:F:841:GLY:O	1:F:842:THR:C	2.60	0.43
1:A:573:SER:O	1:A:575:ALA:N	2.46	0.43
1:A:641:LEU:HG	1:A:659:THR:HB	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:SER:H	1:B:268:ASP:HB3	1.83	0.43
1:B:378:ALA:O	1:B:400:ALA:HB1	2.18	0.43
1:E:581:SER:HA	1:E:602:SER:O	2.18	0.43
1:D:270:PHE:HB3	1:D:296:LEU:HD23	2.00	0.43
1:D:573:SER:HA	1:D:595:ASP:HB3	1.99	0.43
1:F:429:VAL:HG22	1:F:459:VAL:HG13	2.01	0.43
1:F:535:THR:HA	1:F:536:PRO:HD3	1.82	0.43
1:A:581:SER:HA	1:A:602:SER:O	2.18	0.43
1:C:727:GLY:O	1:C:729:THR:HG22	2.18	0.43
1:F:581:SER:HA	1:F:602:SER:O	2.19	0.43
1:B:342:ASN:ND2	1:B:361:THR:HB	2.29	0.43
1:F:250:SER:H	1:F:268:ASP:HB3	1.84	0.43
1:F:378:ALA:O	1:F:400:ALA:HB1	2.17	0.43
1:A:359:ASN:ND2	1:A:378:ALA:HB3	2.34	0.43
1:A:429:VAL:HG22	1:A:459:VAL:HG13	2.00	0.43
1:C:936:SER:O	1:C:936:SER:OG	2.30	0.43
1:E:250:SER:H	1:E:268:ASP:HB3	1.82	0.43
1:E:350:GLN:HE21	1:E:350:GLN:HB2	1.57	0.43
1:E:723:GLY:C	3:E:9101:HOH:O	2.61	0.43
1:A:756:ASN:HB2	1:B:693:PRO:HD2	1.99	0.43
1:B:573:SER:O	1:B:575:ALA:N	2.46	0.43
1:E:727:GLY:O	1:E:729:THR:HG22	2.18	0.43
1:E:1007:LEU:HD23	1:E:1011:VAL:HG11	2.01	0.43
1:B:429:VAL:HG22	1:B:459:VAL:HG13	2.00	0.43
1:B:270:PHE:HB3	1:B:296:LEU:HD23	2.01	0.43
1:F:1007:LEU:HD23	1:F:1011:VAL:HG11	2.00	0.43
1:A:727:GLY:O	1:A:729:THR:HG22	2.18	0.42
1:F:680:LEU:HB2	1:F:698:PHE:CD1	2.54	0.42
1:B:581:SER:HA	1:B:602:SER:O	2.19	0.42
1:D:429:VAL:HG22	1:D:459:VAL:HG13	2.00	0.42
1:D:581:SER:HA	1:D:602:SER:O	2.19	0.42
1:A:693:PRO:HD2	1:B:756:ASN:HB2	2.01	0.42
1:B:308:PRO:HD2	1:B:311:VAL:HG21	2.01	0.42
1:B:727:GLY:O	1:B:729:THR:HG22	2.19	0.42
1:C:350:GLN:HE21	1:C:350:GLN:HB2	1.57	0.42
1:D:727:GLY:O	1:D:729:THR:HG22	2.19	0.42
1:C:680:LEU:HB2	1:C:698:PHE:CD1	2.54	0.42
1:E:367:GLN:HE21	1:E:384:SER:HB3	1.84	0.42
1:E:947:GLY:HA3	1:E:1014:THR:O	2.20	0.42
1:A:687:SER:HB2	1:A:689:PHE:CE1	2.54	0.42
1:A:680:LEU:HB2	1:A:698:PHE:CD1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:THR:HG21	1:B:348:ALA:O	2.20	0.42
1:C:947:GLY:HA3	1:C:1014:THR:O	2.19	0.42
1:A:1007:LEU:HD23	1:A:1011:VAL:HG11	2.02	0.42
1:E:359:ASN:ND2	1:E:378:ALA:HB3	2.35	0.42
1:F:591:ASN:HD22	1:F:612:THR:HB	1.84	0.42
1:A:947:GLY:HA3	1:A:1014:THR:O	2.19	0.42
1:B:947:GLY:HA3	1:B:1014:THR:O	2.19	0.42
1:E:676:GLY:HA2	3:E:9113:HOH:O	2.19	0.42
1:E:680:LEU:HB2	1:E:698:PHE:CD1	2.55	0.42
1:B:680:LEU:HB2	1:B:698:PHE:CD1	2.55	0.42
1:C:516:VAL:HB	1:C:543:LEU:HD12	2.02	0.42
1:F:947:GLY:HA3	1:F:1014:THR:O	2.20	0.42
1:B:567:THR:HG22	1:B:588:THR:HG22	2.02	0.41
1:D:947:GLY:HA3	1:D:1014:THR:O	2.20	0.41
1:E:881:ILE:HA	1:E:899:THR:O	2.20	0.41
1:F:270:PHE:HB3	1:F:296:LEU:HD23	2.00	0.41
1:F:359:ASN:ND2	1:F:378:ALA:HB3	2.35	0.41
1:F:573:SER:O	1:F:575:ALA:N	2.46	0.41
1:D:266:ASN:HD22	1:D:267:ASN:H	1.68	0.41
1:D:1007:LEU:HD23	1:D:1011:VAL:HG11	2.02	0.41
1:E:535:THR:HA	1:E:536:PRO:HD3	1.82	0.41
1:F:727:GLY:O	1:F:729:THR:HG22	2.19	0.41
1:A:270:PHE:HB3	1:A:296:LEU:HD23	2.03	0.41
1:B:967:ALA:HA	1:B:995:ALA:HA	2.02	0.41
1:B:591:ASN:HD22	1:B:612:THR:HB	1.85	0.41
1:D:342:ASN:ND2	1:D:361:THR:HB	2.29	0.41
1:D:680:LEU:HB2	1:D:698:PHE:CD1	2.55	0.41
1:E:342:ASN:ND2	1:E:361:THR:HB	2.29	0.41
1:F:345:THR:HG21	1:F:348:ALA:O	2.20	0.41
1:F:967:ALA:HA	1:F:995:ALA:HA	2.03	0.41
1:B:359:ASN:ND2	1:B:378:ALA:HB3	2.35	0.41
1:C:567:THR:HG22	1:C:588:THR:HG22	2.03	0.41
1:C:958:LEU:HB2	1:C:981:PHE:CE1	2.56	0.41
1:F:266:ASN:HD22	1:F:267:ASN:H	1.69	0.41
1:A:591:ASN:HD22	1:A:612:THR:HB	1.85	0.41
1:A:958:LEU:HB2	1:A:981:PHE:CE1	2.55	0.41
1:B:355:GLY:O	1:B:358:GLN:HG3	2.21	0.41
1:C:359:ASN:ND2	1:C:378:ALA:HB3	2.35	0.41
1:E:687:SER:HB2	1:E:689:PHE:CE1	2.56	0.41
1:A:881:ILE:HA	1:A:899:THR:O	2.21	0.41
1:B:266:ASN:HD22	1:B:267:ASN:H	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:SER:O	1:B:936:SER:OG	2.30	0.41
1:C:881:ILE:HA	1:C:899:THR:O	2.21	0.41
1:D:359:ASN:ND2	1:D:378:ALA:HB3	2.35	0.41
1:D:573:SER:O	1:D:575:ALA:N	2.46	0.41
1:D:881:ILE:HA	1:D:899:THR:O	2.21	0.41
1:E:266:ASN:HD22	1:E:267:ASN:H	1.68	0.41
1:E:270:PHE:HB3	1:E:296:LEU:HD23	2.02	0.41
1:C:681:VAL:HG13	1:C:702:ARG:HG2	2.03	0.41
1:C:967:ALA:HA	1:C:995:ALA:HA	2.03	0.41
1:D:967:ALA:HA	1:D:995:ALA:HA	2.03	0.41
1:A:250:SER:H	1:A:268:ASP:HB3	1.84	0.41
1:A:967:ALA:HA	1:A:995:ALA:HA	2.02	0.41
1:B:535:THR:HA	1:B:536:PRO:HD3	1.82	0.41
1:D:250:SER:O	1:D:268:ASP:CB	2.69	0.41
1:D:591:ASN:HD22	1:D:612:THR:HB	1.85	0.41
1:D:681:VAL:HG13	1:D:702:ARG:HG2	2.03	0.41
1:E:591:ASN:HD22	1:E:612:THR:HB	1.86	0.41
1:E:681:VAL:HG13	1:E:702:ARG:HG2	2.03	0.41
1:F:881:ILE:HA	1:F:899:THR:O	2.20	0.41
1:A:367:GLN:HE21	1:A:384:SER:HB3	1.85	0.41
1:D:567:THR:HG22	1:D:588:THR:HG22	2.03	0.41
1:F:355:GLY:O	1:F:358:GLN:HG3	2.22	0.41
1:F:567:THR:HG22	1:F:588:THR:HG22	2.02	0.41
1:B:597:ARG:HH22	1:B:637:ALA:HB3	1.87	0.40
1:B:1007:LEU:HD23	1:B:1011:VAL:HG11	2.01	0.40
1:D:367:GLN:HE21	1:D:384:SER:HB3	1.85	0.40
1:E:958:LEU:HB2	1:E:981:PHE:CE1	2.56	0.40
1:F:250:SER:O	1:F:268:ASP:CB	2.69	0.40
1:A:681:VAL:HG13	1:A:702:ARG:HG2	2.04	0.40
1:B:687:SER:HB2	1:B:689:PHE:CE1	2.56	0.40
1:C:355:GLY:O	1:C:358:GLN:HG3	2.21	0.40
1:C:951:THR:O	1:C:952:LEU:HD23	2.22	0.40
1:E:516:VAL:HB	1:E:543:LEU:HD12	2.03	0.40
1:B:250:SER:O	1:B:268:ASP:CB	2.69	0.40
1:B:274:GLU:OE1	1:B:277:GLY:HA2	2.22	0.40
1:B:958:LEU:HB2	1:B:981:PHE:CE1	2.57	0.40
1:C:591:ASN:HD22	1:C:612:THR:HB	1.87	0.40
1:E:250:SER:O	1:E:268:ASP:CB	2.70	0.40
1:B:854:THR:HB	1:B:857:GLU:HG3	2.04	0.40
1:C:1007:LEU:HD23	1:C:1011:VAL:HG11	2.03	0.40
1:D:355:GLY:O	1:D:358:GLN:HG3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:681:VAL:HG13	1:F:702:ARG:HG2	2.03	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ASN:ND2	1:D:418:ALA:CB[2_455]	1.49	0.71
1:C:267:ASN:OD1	1:D:418:ALA:CB[2_455]	1.56	0.64
1:C:249:GLY:CA	1:D:391:THR:CG2[2_455]	1.57	0.63
1:C:249:GLY:N	1:D:391:THR:CG2[2_455]	1.60	0.60
1:C:267:ASN:CG	1:D:418:ALA:CB[2_455]	1.60	0.60
1:C:267:ASN:OD1	1:D:418:ALA:N[2_455]	1.77	0.43
1:C:267:ASN:OD1	1:D:418:ALA:CA[2_455]	1.84	0.36
1:C:275:VAL:O	1:F:256:THR:O[2_455]	1.88	0.32

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	A	776/1026 (76%)	709 (91%)	52 (7%)	15 (2%)	6	17
1	B	776/1026 (76%)	710 (92%)	52 (7%)	14 (2%)	6	18
1	C	776/1026 (76%)	711 (92%)	51 (7%)	14 (2%)	6	18
1	D	776/1026 (76%)	710 (92%)	51 (7%)	15 (2%)	6	17
1	E	776/1026 (76%)	712 (92%)	49 (6%)	15 (2%)	6	17
1	F	776/1026 (76%)	712 (92%)	50 (6%)	14 (2%)	6	18
All	All	4656/6156 (76%)	4264 (92%)	305 (7%)	87 (2%)	6	17

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	574	THR
1	A	936	SER
1	A	942	ALA
1	A	1019	ALA
1	B	574	THR
1	B	936	SER
1	B	942	ALA
1	B	1019	ALA
1	C	574	THR
1	C	936	SER
1	C	942	ALA
1	C	1019	ALA
1	D	574	THR
1	D	936	SER
1	D	942	ALA
1	D	1019	ALA
1	E	574	THR
1	E	936	SER
1	E	942	ALA
1	E	1019	ALA
1	F	574	THR
1	F	936	SER
1	F	942	ALA
1	F	1019	ALA
1	A	267	ASN
1	A	667	ALA
1	A	946	PHE
1	A	993	ALA
1	B	267	ASN
1	B	417	GLY
1	B	667	ALA
1	B	946	PHE
1	B	993	ALA
1	C	267	ASN
1	C	667	ALA
1	C	946	PHE
1	C	993	ALA
1	D	267	ASN
1	D	417	GLY
1	D	667	ALA
1	D	946	PHE
1	D	993	ALA
1	E	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	667	ALA
1	E	946	PHE
1	E	993	ALA
1	F	267	ASN
1	F	667	ALA
1	F	946	PHE
1	F	993	ALA
1	A	417	GLY
1	A	502	SER
1	C	417	GLY
1	E	417	GLY
1	F	417	GLY
1	A	378	ALA
1	B	378	ALA
1	B	502	SER
1	B	842	THR
1	C	378	ALA
1	C	502	SER
1	C	842	THR
1	D	378	ALA
1	D	502	SER
1	D	842	THR
1	E	378	ALA
1	E	502	SER
1	E	842	THR
1	F	378	ALA
1	F	502	SER
1	F	842	THR
1	A	665	LEU
1	A	842	THR
1	B	665	LEU
1	D	665	LEU
1	D	1020	THR
1	A	1020	THR
1	C	665	LEU
1	E	665	LEU
1	E	1020	THR
1	F	1020	THR
1	A	668	GLY
1	B	668	GLY
1	C	668	GLY
1	D	668	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	668	GLY
1	F	668	GLY

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	A	526/699 (75%)	467 (89%)	59 (11%)	6	15
1	B	526/699 (75%)	466 (89%)	60 (11%)	5	14
1	C	526/699 (75%)	467 (89%)	59 (11%)	6	15
1	D	526/699 (75%)	469 (89%)	57 (11%)	6	16
1	E	526/699 (75%)	468 (89%)	58 (11%)	6	15
1	F	526/699 (75%)	467 (89%)	59 (11%)	6	15
All	All	3156/4194 (75%)	2804 (89%)	352 (11%)	6	15

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	251	THR
1	A	266	ASN
1	A	275	VAL
1	A	283	VAL
1	A	293	THR
1	A	296	LEU
1	A	299	VAL
1	A	309	THR
1	A	314	SER
1	A	322	THR
1	A	329	LEU
1	A	350	GLN
1	A	358	GLN
1	A	363	THR
1	A	380	VAL
1	A	388	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	393	THR
1	A	429	VAL
1	A	442	THR
1	A	454	THR
1	A	474	ARG
1	A	479	VAL
1	A	490	THR
1	A	491	THR
1	A	494	LYS
1	A	507	THR
1	A	537	THR
1	A	551	THR
1	A	577	SER
1	A	588	THR
1	A	590	LEU
1	A	614	THR
1	A	620	THR
1	A	646	THR
1	A	651	MET
1	A	658	VAL
1	A	662	SER
1	A	671	VAL
1	A	690	SER
1	A	729	THR
1	A	779	VAL
1	A	797	THR
1	A	809	SER
1	A	826	THR
1	A	842	THR
1	A	844	SER
1	A	854	THR
1	A	862	ARG
1	A	873	SER
1	A	875	THR
1	A	892	THR
1	A	906	ILE
1	A	912	ILE
1	A	915	SER
1	A	916	THR
1	A	951	THR
1	A	973	THR
1	A	975	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1012	THR
1	B	251	THR
1	B	266	ASN
1	B	267	ASN
1	B	275	VAL
1	B	283	VAL
1	B	293	THR
1	B	296	LEU
1	B	299	VAL
1	B	309	THR
1	B	314	SER
1	B	322	THR
1	B	329	LEU
1	B	350	GLN
1	B	358	GLN
1	B	363	THR
1	B	380	VAL
1	B	388	THR
1	B	393	THR
1	B	429	VAL
1	B	442	THR
1	B	454	THR
1	B	474	ARG
1	B	479	VAL
1	B	490	THR
1	B	491	THR
1	B	494	LYS
1	B	507	THR
1	B	537	THR
1	B	551	THR
1	B	577	SER
1	B	588	THR
1	B	590	LEU
1	B	614	THR
1	B	620	THR
1	B	646	THR
1	B	651	MET
1	B	658	VAL
1	B	662	SER
1	B	671	VAL
1	B	690	SER
1	B	729	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	779	VAL
1	B	797	THR
1	B	809	SER
1	B	826	THR
1	B	842	THR
1	B	844	SER
1	B	854	THR
1	B	862	ARG
1	B	873	SER
1	B	875	THR
1	B	892	THR
1	B	906	ILE
1	B	912	ILE
1	B	915	SER
1	B	916	THR
1	B	951	THR
1	B	973	THR
1	B	975	VAL
1	B	1012	THR
1	C	251	THR
1	C	266	ASN
1	C	267	ASN
1	C	275	VAL
1	C	283	VAL
1	C	293	THR
1	C	296	LEU
1	C	299	VAL
1	C	307	LEU
1	C	309	THR
1	C	314	SER
1	C	322	THR
1	C	329	LEU
1	C	350	GLN
1	C	358	GLN
1	C	363	THR
1	C	380	VAL
1	C	388	THR
1	C	393	THR
1	C	429	VAL
1	C	442	THR
1	C	454	THR
1	C	474	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	479	VAL
1	C	490	THR
1	C	491	THR
1	C	494	LYS
1	C	537	THR
1	C	551	THR
1	C	577	SER
1	C	588	THR
1	C	590	LEU
1	C	614	THR
1	C	620	THR
1	C	646	THR
1	C	651	MET
1	C	658	VAL
1	C	662	SER
1	C	671	VAL
1	C	690	SER
1	C	729	THR
1	C	779	VAL
1	C	797	THR
1	C	809	SER
1	C	826	THR
1	C	842	THR
1	C	844	SER
1	C	862	ARG
1	C	873	SER
1	C	875	THR
1	C	892	THR
1	C	906	ILE
1	C	912	ILE
1	C	915	SER
1	C	916	THR
1	C	951	THR
1	C	973	THR
1	C	975	VAL
1	C	1012	THR
1	D	251	THR
1	D	266	ASN
1	D	275	VAL
1	D	283	VAL
1	D	293	THR
1	D	296	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	299	VAL
1	D	309	THR
1	D	314	SER
1	D	322	THR
1	D	329	LEU
1	D	350	GLN
1	D	358	GLN
1	D	363	THR
1	D	380	VAL
1	D	388	THR
1	D	393	THR
1	D	429	VAL
1	D	442	THR
1	D	454	THR
1	D	474	ARG
1	D	479	VAL
1	D	490	THR
1	D	491	THR
1	D	494	LYS
1	D	507	THR
1	D	537	THR
1	D	551	THR
1	D	577	SER
1	D	588	THR
1	D	590	LEU
1	D	614	THR
1	D	620	THR
1	D	646	THR
1	D	651	MET
1	D	658	VAL
1	D	662	SER
1	D	671	VAL
1	D	690	SER
1	D	729	THR
1	D	779	VAL
1	D	797	THR
1	D	809	SER
1	D	826	THR
1	D	842	THR
1	D	844	SER
1	D	862	ARG
1	D	873	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	875	THR
1	D	892	THR
1	D	906	ILE
1	D	915	SER
1	D	916	THR
1	D	951	THR
1	D	973	THR
1	D	975	VAL
1	D	1012	THR
1	E	251	THR
1	E	266	ASN
1	E	275	VAL
1	E	283	VAL
1	E	293	THR
1	E	296	LEU
1	E	299	VAL
1	E	309	THR
1	E	314	SER
1	E	322	THR
1	E	329	LEU
1	E	350	GLN
1	E	358	GLN
1	E	363	THR
1	E	380	VAL
1	E	388	THR
1	E	393	THR
1	E	429	VAL
1	E	442	THR
1	E	454	THR
1	E	474	ARG
1	E	479	VAL
1	E	490	THR
1	E	491	THR
1	E	494	LYS
1	E	537	THR
1	E	551	THR
1	E	577	SER
1	E	588	THR
1	E	590	LEU
1	E	614	THR
1	E	620	THR
1	E	646	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	651	MET
1	E	658	VAL
1	E	662	SER
1	E	671	VAL
1	E	690	SER
1	E	729	THR
1	E	779	VAL
1	E	797	THR
1	E	809	SER
1	E	826	THR
1	E	842	THR
1	E	844	SER
1	E	854	THR
1	E	862	ARG
1	E	873	SER
1	E	875	THR
1	E	892	THR
1	E	906	ILE
1	E	912	ILE
1	E	915	SER
1	E	916	THR
1	E	951	THR
1	E	973	THR
1	E	975	VAL
1	E	1012	THR
1	F	251	THR
1	F	266	ASN
1	F	275	VAL
1	F	283	VAL
1	F	293	THR
1	F	296	LEU
1	F	299	VAL
1	F	309	THR
1	F	314	SER
1	F	322	THR
1	F	329	LEU
1	F	350	GLN
1	F	358	GLN
1	F	363	THR
1	F	380	VAL
1	F	388	THR
1	F	393	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	429	VAL
1	F	442	THR
1	F	454	THR
1	F	474	ARG
1	F	479	VAL
1	F	490	THR
1	F	491	THR
1	F	494	LYS
1	F	537	THR
1	F	551	THR
1	F	577	SER
1	F	588	THR
1	F	590	LEU
1	F	614	THR
1	F	620	THR
1	F	646	THR
1	F	651	MET
1	F	658	VAL
1	F	662	SER
1	F	671	VAL
1	F	690	SER
1	F	729	THR
1	F	779	VAL
1	F	797	THR
1	F	809	SER
1	F	826	THR
1	F	842	THR
1	F	844	SER
1	F	854	THR
1	F	858	VAL
1	F	862	ARG
1	F	873	SER
1	F	875	THR
1	F	892	THR
1	F	906	ILE
1	F	912	ILE
1	F	915	SER
1	F	916	THR
1	F	951	THR
1	F	973	THR
1	F	975	VAL
1	F	1012	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	ASN
1	A	267	ASN
1	A	342	ASN
1	A	350	GLN
1	A	358	GLN
1	A	359	ASN
1	A	367	GLN
1	A	371	ASN
1	A	476	ASN
1	A	672	ASN
1	A	709	GLN
1	A	938	ASN
1	B	266	ASN
1	B	267	ASN
1	B	342	ASN
1	B	344	ASN
1	B	350	GLN
1	B	358	GLN
1	B	359	ASN
1	B	367	GLN
1	B	371	ASN
1	B	476	ASN
1	B	672	ASN
1	B	709	GLN
1	B	938	ASN
1	C	266	ASN
1	C	267	ASN
1	C	342	ASN
1	C	344	ASN
1	C	350	GLN
1	C	358	GLN
1	C	359	ASN
1	C	367	GLN
1	C	371	ASN
1	C	672	ASN
1	C	709	GLN
1	C	938	ASN
1	D	266	ASN
1	D	267	ASN
1	D	342	ASN
1	D	350	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	358	GLN
1	D	359	ASN
1	D	367	GLN
1	D	371	ASN
1	D	476	ASN
1	D	672	ASN
1	D	709	GLN
1	D	715	ASN
1	D	938	ASN
1	E	266	ASN
1	E	267	ASN
1	E	342	ASN
1	E	344	ASN
1	E	350	GLN
1	E	358	GLN
1	E	359	ASN
1	E	367	GLN
1	E	371	ASN
1	E	476	ASN
1	E	591	ASN
1	E	672	ASN
1	E	709	GLN
1	E	938	ASN
1	F	266	ASN
1	F	267	ASN
1	F	342	ASN
1	F	344	ASN
1	F	350	GLN
1	F	358	GLN
1	F	359	ASN
1	F	367	GLN
1	F	371	ASN
1	F	476	ASN
1	F	672	ASN
1	F	709	GLN
1	F	938	ASN

5.3.3 RNA ⓘ

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 114 ligands modelled in this entry, 114 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 ⓘ

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	A	778/1026 (75%)	0.22	23 (2%)	52	49	7, 16, 52, 102	0
1	B	778/1026 (75%)	0.35	30 (3%)	43	39	9, 21, 46, 97	0
1	C	778/1026 (75%)	0.50	28 (3%)	46	42	11, 22, 46, 140	0
1	D	778/1026 (75%)	0.42	24 (3%)	51	48	9, 20, 40, 92	0
1	E	778/1026 (75%)	0.40	32 (4%)	41	37	9, 22, 45, 85	0
1	F	778/1026 (75%)	0.31	37 (4%)	35	32	9, 18, 48, 94	0
All	All	4668/6156 (75%)	0.37	174 (3%)	45	41	7, 20, 46, 140	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	GLY	8.1
1	B	946	PHE	7.8
1	F	946	PHE	7.4
1	C	250	SER	7.2
1	A	946	PHE	7.0
1	D	946	PHE	6.9
1	E	292	GLY	6.8
1	D	292	GLY	6.6
1	B	971	SER	6.2
1	C	249	GLY	5.8
1	F	292	GLY	5.8
1	C	267	ASN	5.6
1	C	946	PHE	5.3
1	A	293	THR	5.1
1	E	946	PHE	5.1
1	C	276	ALA	5.1
1	C	251	THR	5.0
1	F	267	ASN	5.0
1	F	293	THR	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	942	ALA	4.7
1	C	292	GLY	4.5
1	D	266	ASN	4.5
1	D	942	ALA	4.4
1	B	267	ASN	4.4
1	D	249	GLY	4.4
1	D	267	ASN	4.3
1	E	492	ALA	4.2
1	F	941	ILE	4.1
1	D	945	ALA	3.9
1	F	842	THR	3.9
1	A	973	THR	3.9
1	C	942	ALA	3.8
1	E	842	THR	3.7
1	B	972	GLY	3.7
1	F	968	GLY	3.6
1	F	967	ALA	3.5
1	C	275	VAL	3.5
1	F	1019	ALA	3.5
1	F	1020	THR	3.3
1	E	293	THR	3.3
1	A	842	THR	3.3
1	C	912	ILE	3.3
1	D	690	SER	3.2
1	F	973	THR	3.2
1	C	842	THR	3.1
1	C	291	ALA	3.1
1	B	842	THR	3.1
1	A	912	ILE	3.1
1	B	973	THR	3.1
1	D	564	GLY	3.0
1	A	970	GLY	3.0
1	A	1022	VAL	3.0
1	C	333	SER	2.9
1	E	995	ALA	2.9
1	B	293	THR	2.9
1	B	916	THR	2.9
1	A	975	VAL	2.9
1	B	264	THR	2.8
1	C	855	VAL	2.8
1	A	971	SER	2.8
1	B	969	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	492	ALA	2.8
1	D	251	THR	2.8
1	F	996	THR	2.8
1	B	564	GLY	2.7
1	F	972	GLY	2.7
1	C	1020	THR	2.7
1	F	969	ASP	2.7
1	A	530	GLY	2.7
1	B	292	GLY	2.7
1	C	973	THR	2.7
1	B	975	VAL	2.6
1	E	1019	ALA	2.6
1	F	971	SER	2.6
1	B	1020	THR	2.6
1	E	970	GLY	2.6
1	C	690	SER	2.6
1	A	267	ASN	2.6
1	B	492	ALA	2.6
1	B	561	ALA	2.6
1	B	942	ALA	2.6
1	B	1019	ALA	2.6
1	E	606	ALA	2.5
1	E	667	ALA	2.5
1	D	753	THR	2.5
1	E	396	ALA	2.5
1	F	976	ALA	2.5
1	B	1015	THR	2.5
1	F	291	ALA	2.5
1	F	993	ALA	2.5
1	A	996	THR	2.4
1	E	968	GLY	2.4
1	B	667	ALA	2.4
1	C	1018	PHE	2.4
1	B	276	ALA	2.4
1	C	1019	ALA	2.4
1	D	691	ALA	2.4
1	E	561	ALA	2.4
1	F	995	ALA	2.4
1	A	914	THR	2.3
1	F	963	ASP	2.3
1	C	964	ALA	2.3
1	E	531	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	940	ALA	2.3
1	E	912	ILE	2.3
1	E	690	SER	2.3
1	E	528	GLY	2.3
1	E	530	GLY	2.3
1	A	949	ALA	2.3
1	C	293	THR	2.3
1	D	268	ASP	2.3
1	F	249	GLY	2.3
1	F	994	GLY	2.3
1	B	307	LEU	2.3
1	A	976	ALA	2.3
1	C	995	ALA	2.3
1	E	942	ALA	2.3
1	F	937	THR	2.3
1	A	1019	ALA	2.2
1	C	534	ALA	2.2
1	D	559	ALA	2.2
1	C	796	THR	2.2
1	C	996	THR	2.2
1	E	414	THR	2.2
1	F	551	THR	2.2
1	C	670	SER	2.2
1	F	936	SER	2.2
1	E	357	GLY	2.2
1	F	1018	PHE	2.2
1	D	967	ALA	2.2
1	E	538	ALA	2.2
1	A	551	THR	2.2
1	A	916	THR	2.2
1	D	760	THR	2.2
1	E	685	ASN	2.2
1	A	998	VAL	2.2
1	F	975	VAL	2.2
1	D	265	ALA	2.2
1	A	892	THR	2.2
1	B	249	GLY	2.2
1	D	944	GLY	2.2
1	F	530	GLY	2.2
1	E	975	VAL	2.2
1	D	418	ALA	2.2
1	F	954	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	414	THR	2.1
1	F	947	GLY	2.1
1	F	970	GLY	2.1
1	B	275	VAL	2.1
1	C	906	ILE	2.1
1	E	971	SER	2.1
1	B	356	ALA	2.1
1	E	967	ALA	2.1
1	B	840	THR	2.1
1	D	646	THR	2.1
1	E	1020	THR	2.1
1	D	356	ALA	2.1
1	C	266	ASN	2.1
1	D	594	GLY	2.1
1	E	753	THR	2.1
1	A	1000	GLY	2.1
1	B	947	GLY	2.1
1	F	943	ASP	2.0
1	A	886	ALA	2.0
1	E	356	ALA	2.0
1	E	973	THR	2.0
1	E	944	GLY	2.0
1	F	998	VAL	2.0
1	D	667	ALA	2.0
1	F	265	ALA	2.0
1	F	538	ALA	2.0
1	B	796	THR	2.0
1	B	1014	THR	2.0
1	E	668	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
2	CA	F	9017	1/1	0.80	0.18	90,90,90,90	0
2	CA	E	9004	1/1	0.81	0.09	49,49,49,49	0
2	CA	A	9018	1/1	0.81	0.32	98,98,98,98	0
2	CA	E	9018	1/1	0.83	0.31	105,105,105,105	0
2	CA	B	9018	1/1	0.85	0.36	95,95,95,95	0
2	CA	F	9018	1/1	0.85	0.30	109,109,109,109	0
2	CA	B	9017	1/1	0.87	0.10	59,59,59,59	0
2	CA	E	9017	1/1	0.88	0.10	33,33,33,33	0
2	CA	D	9018	1/1	0.88	0.15	81,81,81,81	0
2	CA	A	9017	1/1	0.89	0.12	80,80,80,80	0
2	CA	F	9015	1/1	0.89	0.06	48,48,48,48	0
2	CA	C	9019	1/1	0.90	0.12	97,97,97,97	0
2	CA	E	9001	1/1	0.90	0.06	42,42,42,42	0
2	CA	E	9016	1/1	0.91	0.06	34,34,34,34	0
2	CA	C	9004	1/1	0.92	0.06	32,32,32,32	0
2	CA	B	9001	1/1	0.92	0.06	25,25,25,25	0
2	CA	D	9017	1/1	0.92	0.07	37,37,37,37	0
2	CA	B	9010	1/1	0.92	0.06	27,27,27,27	0
2	CA	F	9019	1/1	0.92	0.09	61,61,61,61	0
2	CA	B	9002	1/1	0.93	0.07	43,43,43,43	0
2	CA	C	9017	1/1	0.93	0.15	78,78,78,78	0
2	CA	C	9018	1/1	0.93	0.16	82,82,82,82	0
2	CA	B	9019	1/1	0.94	0.07	51,51,51,51	0
2	CA	F	9001	1/1	0.94	0.06	27,27,27,27	0
2	CA	F	9010	1/1	0.94	0.07	30,30,30,30	0
2	CA	A	9001	1/1	0.94	0.07	15,15,15,15	0
2	CA	E	9010	1/1	0.94	0.06	44,44,44,44	0
2	CA	C	9010	1/1	0.94	0.07	39,39,39,39	0
2	CA	B	9016	1/1	0.94	0.04	31,31,31,31	0
2	CA	D	9005	1/1	0.95	0.06	23,23,23,23	0
2	CA	D	9010	1/1	0.95	0.05	44,44,44,44	0
2	CA	C	9016	1/1	0.95	0.04	18,18,18,18	0
2	CA	A	9010	1/1	0.95	0.07	30,30,30,30	0
2	CA	F	9002	1/1	0.95	0.06	17,17,17,17	0
2	CA	F	9005	1/1	0.95	0.05	29,29,29,29	0
2	CA	D	9019	1/1	0.95	0.04	27,27,27,27	0
2	CA	C	9005	1/1	0.95	0.04	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	F	9016	1/1	0.95	0.05	22,22,22,22	0
2	CA	E	9002	1/1	0.95	0.04	43,43,43,43	0
2	CA	C	9002	1/1	0.95	0.06	29,29,29,29	0
2	CA	D	9004	1/1	0.95	0.05	42,42,42,42	0
2	CA	A	9013	1/1	0.96	0.04	20,20,20,20	0
2	CA	D	9012	1/1	0.96	0.04	21,21,21,21	0
2	CA	F	9004	1/1	0.96	0.05	36,36,36,36	0
2	CA	D	9013	1/1	0.96	0.06	33,33,33,33	0
2	CA	F	9009	1/1	0.96	0.03	14,14,14,14	0
2	CA	E	9005	1/1	0.96	0.04	26,26,26,26	0
2	CA	D	9015	1/1	0.96	0.04	31,31,31,31	0
2	CA	E	9015	1/1	0.96	0.05	46,46,46,46	0
2	CA	D	9002	1/1	0.96	0.06	30,30,30,30	0
2	CA	C	9006	1/1	0.96	0.03	26,26,26,26	0
2	CA	B	9015	1/1	0.96	0.05	47,47,47,47	0
2	CA	C	9008	1/1	0.97	0.04	29,29,29,29	0
2	CA	C	9009	1/1	0.97	0.04	28,28,28,28	0
2	CA	A	9004	1/1	0.97	0.04	19,19,19,19	0
2	CA	C	9013	1/1	0.97	0.03	35,35,35,35	0
2	CA	A	9014	1/1	0.97	0.04	32,32,32,32	0
2	CA	B	9004	1/1	0.97	0.05	25,25,25,25	0
2	CA	B	9005	1/1	0.97	0.04	35,35,35,35	0
2	CA	B	9007	1/1	0.97	0.05	16,16,16,16	0
2	CA	D	9001	1/1	0.97	0.04	31,31,31,31	0
2	CA	A	9005	1/1	0.97	0.03	14,14,14,14	0
2	CA	F	9013	1/1	0.97	0.02	16,16,16,16	0
2	CA	B	9013	1/1	0.97	0.03	19,19,19,19	0
2	CA	E	9006	1/1	0.97	0.03	26,26,26,26	0
2	CA	E	9007	1/1	0.97	0.04	23,23,23,23	0
2	CA	A	9002	1/1	0.97	0.05	18,18,18,18	0
2	CA	E	9013	1/1	0.97	0.05	30,30,30,30	0
2	CA	D	9014	1/1	0.98	0.04	26,26,26,26	0
2	CA	C	9007	1/1	0.98	0.04	21,21,21,21	0
2	CA	D	9016	1/1	0.98	0.02	23,23,23,23	0
2	CA	A	9006	1/1	0.98	0.03	20,20,20,20	0
2	CA	E	9019	1/1	0.98	0.06	67,67,67,67	0
2	CA	C	9001	1/1	0.98	0.04	23,23,23,23	0
2	CA	A	9019	1/1	0.98	0.04	39,39,39,39	0
2	CA	D	9003	1/1	0.98	0.02	9,9,9,9	0
2	CA	A	9015	1/1	0.98	0.03	42,42,42,42	0
2	CA	C	9014	1/1	0.98	0.05	20,20,20,20	0
2	CA	D	9006	1/1	0.98	0.04	22,22,22,22	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	D	9008	1/1	0.98	0.04	36,36,36,36	0
2	CA	C	9015	1/1	0.98	0.03	39,39,39,39	0
2	CA	B	9008	1/1	0.98	0.03	22,22,22,22	0
2	CA	E	9011	1/1	0.98	0.02	29,29,29,29	0
2	CA	A	9009	1/1	0.98	0.03	11,11,11,11	0
2	CA	E	9014	1/1	0.98	0.05	22,22,22,22	0
2	CA	C	9011	1/1	0.99	0.06	21,21,21,21	0
2	CA	D	9009	1/1	0.99	0.02	15,15,15,15	0
2	CA	E	9012	1/1	0.99	0.01	20,20,20,20	0
2	CA	C	9012	1/1	0.99	0.02	26,26,26,26	0
2	CA	D	9011	1/1	0.99	0.02	23,23,23,23	0
2	CA	A	9011	1/1	0.99	0.03	17,17,17,17	0
2	CA	B	9006	1/1	0.99	0.02	17,17,17,17	0
2	CA	A	9012	1/1	0.99	0.02	19,19,19,19	0
2	CA	A	9008	1/1	0.99	0.04	11,11,11,11	0
2	CA	B	9009	1/1	0.99	0.02	9,9,9,9	0
2	CA	C	9003	1/1	0.99	0.02	15,15,15,15	0
2	CA	A	9003	1/1	0.99	0.02	10,10,10,10	0
2	CA	B	9011	1/1	0.99	0.03	18,18,18,18	0
2	CA	B	9012	1/1	0.99	0.02	26,26,26,26	0
2	CA	F	9007	1/1	0.99	0.06	27,27,27,27	0
2	CA	F	9008	1/1	0.99	0.03	11,11,11,11	0
2	CA	A	9007	1/1	0.99	0.04	17,17,17,17	0
2	CA	E	9003	1/1	0.99	0.04	13,13,13,13	0
2	CA	F	9011	1/1	0.99	0.04	44,44,44,44	0
2	CA	F	9012	1/1	0.99	0.03	19,19,19,19	0
2	CA	B	9014	1/1	0.99	0.03	31,31,31,31	0
2	CA	F	9014	1/1	0.99	0.03	12,12,12,12	0
2	CA	B	9003	1/1	0.99	0.02	17,17,17,17	0
2	CA	A	9016	1/1	0.99	0.03	13,13,13,13	0
2	CA	D	9007	1/1	0.99	0.04	14,14,14,14	0
2	CA	E	9008	1/1	0.99	0.03	18,18,18,18	0
2	CA	E	9009	1/1	0.99	0.03	12,12,12,12	0
2	CA	F	9006	1/1	1.00	0.03	9,9,9,9	0
2	CA	F	9003	1/1	1.00	0.02	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.