



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 04:54 am BST

PDB ID : 6P5T
Title : Surface-layer (S-layer) RsaA protein from *Caulobacter crescentus* bound to strontium and iodide
Authors : Chan, A.C.; Herrmann, J.; Smit, J.; Wakatsuki, S.; Murphy, M.E.
Deposited on : 2019-05-30
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

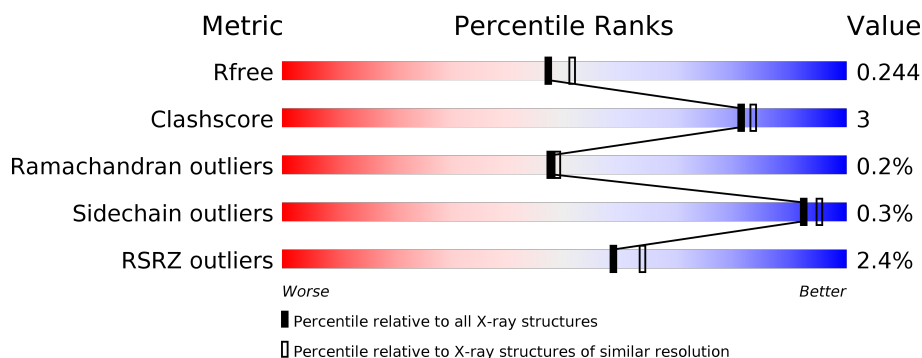
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 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	814	<div> <div>93%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	B	814	<div> <div>5%</div> <div>91%</div> <div>5%</div> <div>5%</div> </div>
1	C	814	<div> <div>5%</div> <div>90%</div> <div>6%</div> <div></div> </div>
1	D	814	<div> <div>2%</div> <div>90%</div> <div>5%</div> <div></div> </div>
1	E	814	<div> <div>2%</div> <div>90%</div> <div>6%</div> <div></div> </div>
1	F	814	<div> <div>3%</div> <div>90%</div> <div>6%</div> <div></div> </div>

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
2	IOD	A	1128	-	-	X	-
2	IOD	B	1116	-	-	X	-
2	IOD	B	1117	-	-	X	-
2	IOD	C	1110	-	-	X	-
2	IOD	D	1119	-	-	X	-
2	IOD	E	1122	-	-	X	-
2	IOD	F	1127	-	-	X	-
2	IOD	F	1130	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36028 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	782	Total	C	N	O	S	0	1	0
			5162	3140	867	1153	2			
1	B	776	Total	C	N	O	S	0	2	0
			5135	3125	862	1146	2			
1	C	781	Total	C	N	O	S	0	1	0
			5156	3137	866	1151	2			
1	D	780	Total	C	N	O	S	0	1	0
			5152	3135	865	1150	2			
1	E	781	Total	C	N	O	S	0	0	0
			5150	3134	865	1149	2			
1	F	782	Total	C	N	O	S	0	1	0
			5162	3140	867	1153	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	MET	-	initiating methionine	UNP P35828
A	214	THR	-	expression tag	UNP P35828
A	215	MET	-	expression tag	UNP P35828
A	216	ILE	-	expression tag	UNP P35828
A	217	THR	-	expression tag	UNP P35828
A	218	ASN	-	expression tag	UNP P35828
A	219	SER	-	expression tag	UNP P35828
A	220	ARG	-	expression tag	UNP P35828
A	221	GLY	-	expression tag	UNP P35828
A	222	SER	-	expression tag	UNP P35828
B	213	MET	-	initiating methionine	UNP P35828
B	214	THR	-	expression tag	UNP P35828
B	215	MET	-	expression tag	UNP P35828
B	216	ILE	-	expression tag	UNP P35828
B	217	THR	-	expression tag	UNP P35828
B	218	ASN	-	expression tag	UNP P35828
B	219	SER	-	expression tag	UNP P35828

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Chain	Residue	Modelled	Actual	Comment	Reference
B	220	ARG	-	expression tag	UNP P35828
B	221	GLY	-	expression tag	UNP P35828
B	222	SER	-	expression tag	UNP P35828
C	213	MET	-	initiating methionine	UNP P35828
C	214	THR	-	expression tag	UNP P35828
C	215	MET	-	expression tag	UNP P35828
C	216	ILE	-	expression tag	UNP P35828
C	217	THR	-	expression tag	UNP P35828
C	218	ASN	-	expression tag	UNP P35828
C	219	SER	-	expression tag	UNP P35828
C	220	ARG	-	expression tag	UNP P35828
C	221	GLY	-	expression tag	UNP P35828
C	222	SER	-	expression tag	UNP P35828
D	213	MET	-	initiating methionine	UNP P35828
D	214	THR	-	expression tag	UNP P35828
D	215	MET	-	expression tag	UNP P35828
D	216	ILE	-	expression tag	UNP P35828
D	217	THR	-	expression tag	UNP P35828
D	218	ASN	-	expression tag	UNP P35828
D	219	SER	-	expression tag	UNP P35828
D	220	ARG	-	expression tag	UNP P35828
D	221	GLY	-	expression tag	UNP P35828
D	222	SER	-	expression tag	UNP P35828
E	213	MET	-	initiating methionine	UNP P35828
E	214	THR	-	expression tag	UNP P35828
E	215	MET	-	expression tag	UNP P35828
E	216	ILE	-	expression tag	UNP P35828
E	217	THR	-	expression tag	UNP P35828
E	218	ASN	-	expression tag	UNP P35828
E	219	SER	-	expression tag	UNP P35828
E	220	ARG	-	expression tag	UNP P35828
E	221	GLY	-	expression tag	UNP P35828
E	222	SER	-	expression tag	UNP P35828
F	213	MET	-	initiating methionine	UNP P35828
F	214	THR	-	expression tag	UNP P35828
F	215	MET	-	expression tag	UNP P35828
F	216	ILE	-	expression tag	UNP P35828
F	217	THR	-	expression tag	UNP P35828
F	218	ASN	-	expression tag	UNP P35828
F	219	SER	-	expression tag	UNP P35828
F	220	ARG	-	expression tag	UNP P35828
F	221	GLY	-	expression tag	UNP P35828

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Chain	Residue	Modelled	Actual	Comment	Reference
F	222	SER	-	expression tag	UNP P35828

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	23	Total I 23 23	0	0
2	E	24	Total I 24 24	0	0
2	B	24	Total I 24 24	0	0
2	C	20	Total I 20 20	0	0
2	A	29	Total I 29 29	0	0
2	F	30	Total I 30 30	0	0

- Molecule 3 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	19	Total Sr 19 19	0	0
3	E	21	Total Sr 21 21	0	0
3	B	20	Total Sr 20 20	0	0
3	C	21	Total Sr 21 21	0	0
3	A	20	Total Sr 20 20	0	0
3	F	23	Total Sr 23 23	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1058	Total O 1058 1058	0	0
4	B	924	Total O 924 924	0	0

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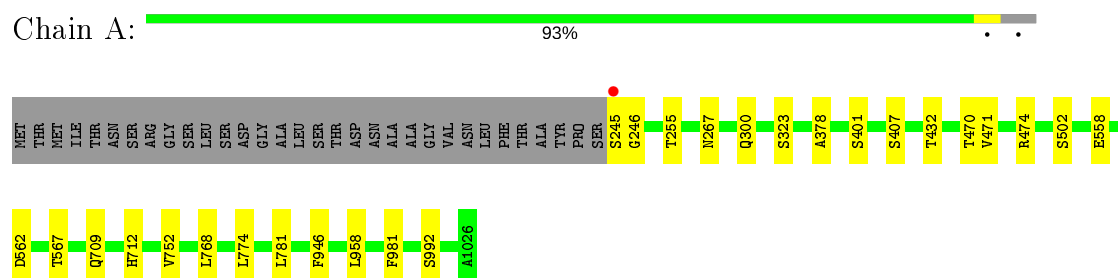
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	599	Total 599	O 599	0	0
4	D	690	Total 690	O 690	0	0
4	E	730	Total 730	O 730	0	0
4	F	836	Total 836	O 836	0	0

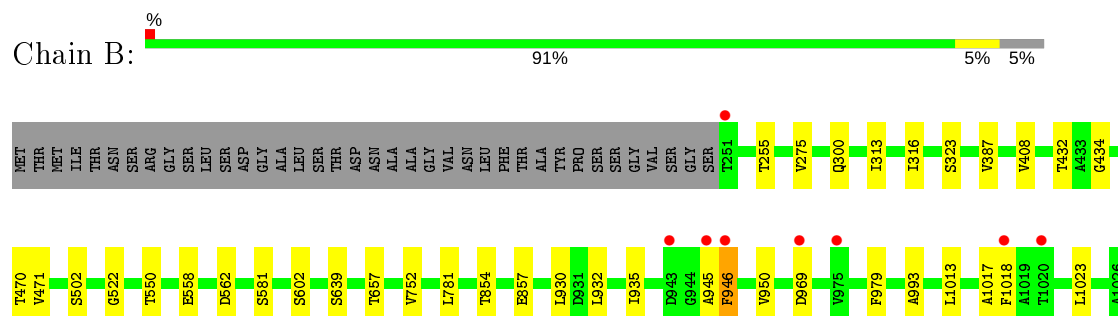
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

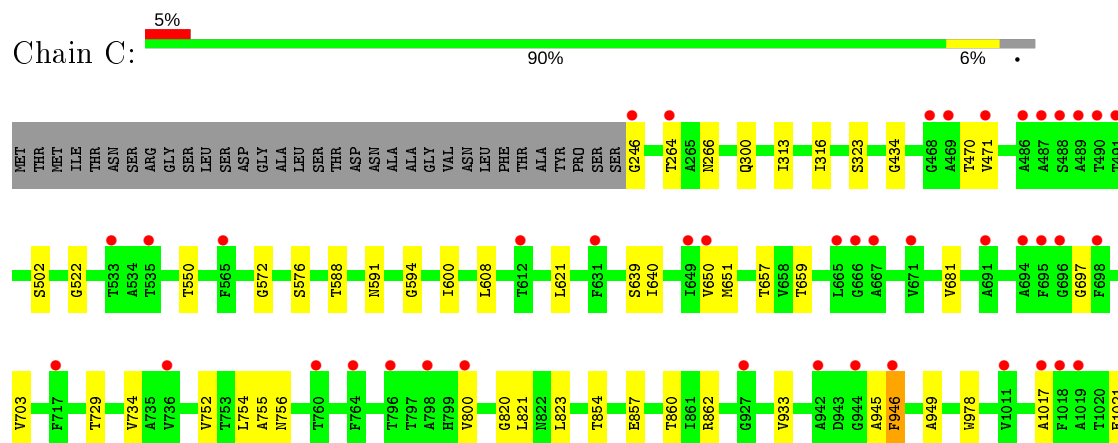
- Molecule 1: S-layer protein



- Molecule 1: S-layer protein

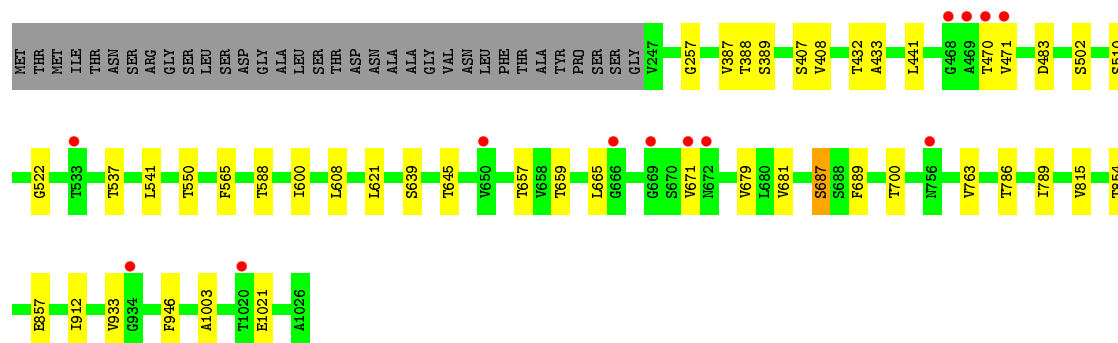


- Molecule 1: S-layer protein

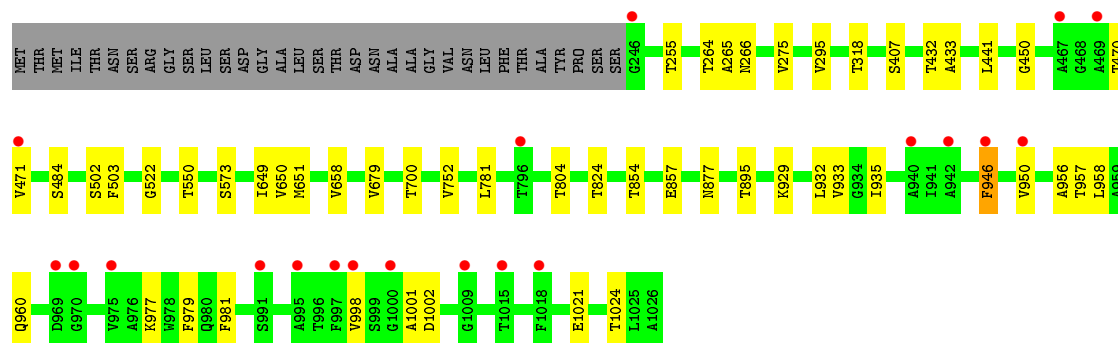
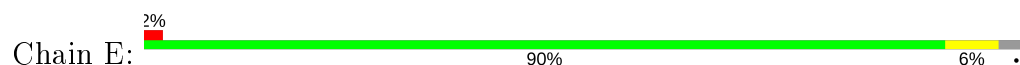




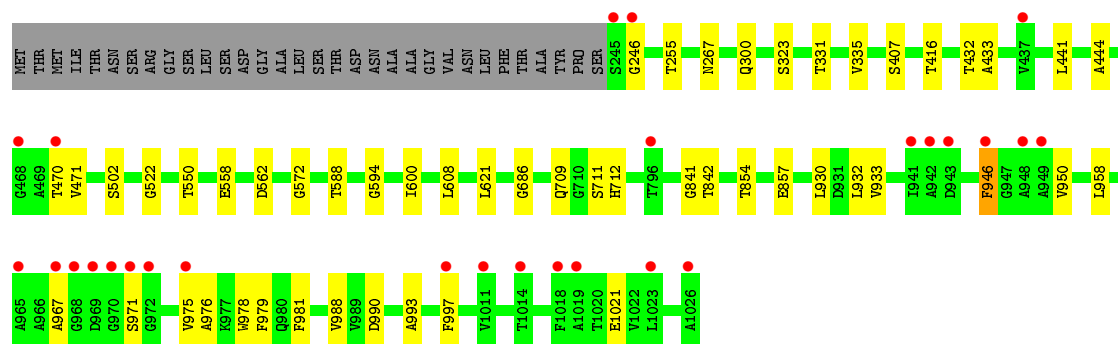
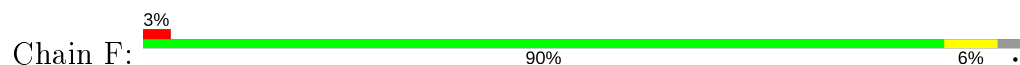
• Molecule 1: S-layer protein



• Molecule 1: S-layer protein



• Molecule 1: S-layer protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	210.73 Å 80.56 Å 221.83 Å 90.00° 117.44° 90.00°	Depositor
Resolution (Å)	49.30 – 2.10 49.30 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.30-2.10) 99.8 (49.30-2.10)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.10 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.205 , 0.243 0.208 , 0.244	Depositor DCC
R_{free} test set	19236 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	1.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36028	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 29.33 % 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 1.5780e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.33	0/5195	0.58	0/7151
1	B	0.33	0/5168	0.57	0/7115
1	C	0.31	0/5189	0.57	0/7143
1	D	0.31	0/5185	0.56	0/7138
1	E	0.31	0/5183	0.56	0/7135
1	F	0.33	0/5195	0.57	0/7151
All	All	0.32	0/31115	0.57	0/42833

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5162	0	5096	17	0
1	B	5135	0	5070	22	0
1	C	5156	0	5090	32	0
1	D	5152	0	5088	23	0
1	E	5150	0	5086	32	0
1	F	5162	0	5096	29	0
2	A	29	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	24	0	0	5	0
2	C	20	0	0	3	0
2	D	23	0	0	3	0
2	E	24	0	0	5	0
2	F	30	0	0	6	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	21	0	0	0	0
3	D	19	0	0	0	0
3	E	21	0	0	0	0
3	F	23	0	0	0	0
4	A	1058	0	0	2	0
4	B	924	0	0	1	0
4	C	599	0	0	5	0
4	D	690	0	0	0	0
4	E	730	0	0	1	0
4	F	836	0	0	1	0
All	All	36028	0	30526	160	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 3.

All (160) 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:B:1113:IOD:I	2:B:1116:IOD:I	3.25	0.94
2:D:1109:IOD:I	2:D:1110:IOD:I	3.28	0.92
2:A:1116:IOD:I	2:A:1119:IOD:I	3.31	0.89
2:F:1116:IOD:I	2:F:1117:IOD:I	3.31	0.88
1:E:650:VAL:HG13	2:E:1103:IOD:I	2.43	0.88
2:C:1109:IOD:I	2:C:1110:IOD:I	3.35	0.85
1:C:650:VAL:HG13	2:C:1105:IOD:I	2.48	0.83
2:E:1110:IOD:I	2:E:1115:IOD:I	3.39	0.81
1:F:930:LEU:HG	1:F:932:LEU:HD21	1.68	0.75
1:A:432:THR:HG23	2:A:1128:IOD:I	2.62	0.69
1:E:956:ALA:HA	1:E:960:GLN:HE21	1.57	0.68
1:A:245:SER:HA	1:A:267:ASN:HD21	1.58	0.67
1:E:295:VAL:HG22	1:E:318:THR:HB	1.77	0.66
1:F:470:THR:HG23	1:F:471:VAL:HG13	1.76	0.66
1:D:470:THR:HG23	1:D:471:VAL:HG23	1.80	0.63
1:F:432:THR:HG23	2:F:1127:IOD:I	2.69	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:842:THR:HG23	2:F:1130:IOD:I	2.68	0.62
1:D:407:SER:HB3	2:D:1119:IOD:I	2.70	0.61
1:D:483:ASP:HB2	1:D:510:SER:HB2	1.82	0.61
1:E:407:SER:HB3	2:E:1122:IOD:I	2.72	0.60
1:E:432:THR:HG23	2:E:1122:IOD:I	2.71	0.60
1:B:470:THR:HG23	1:B:471:VAL:HG23	1.83	0.59
1:B:432:THR:HG23	2:B:1121:IOD:I	2.72	0.59
1:C:754:LEU:HD22	1:C:756:ASN:H	1.68	0.59
1:E:854:THR:OG1	1:E:857:GLU:HB2	2.03	0.59
1:E:998:VAL:HG13	1:E:1001:ALA:HB3	1.87	0.57
1:F:407:SER:HB3	2:F:1127:IOD:I	2.75	0.56
1:C:470:THR:HG23	1:C:471:VAL:HG23	1.86	0.56
1:C:754:LEU:HD23	1:C:755:ALA:H	1.70	0.56
1:B:854:THR:HB	1:B:857:GLU:HB2	1.86	0.56
1:D:600:ILE:HB	1:D:621:LEU:HD13	1.89	0.55
1:C:600:ILE:HB	1:C:621:LEU:HD23	1.89	0.54
1:E:932:LEU:HD22	1:E:935:ILE:HD11	1.89	0.54
1:C:659:THR:HA	1:C:681:VAL:HB	1.90	0.54
1:F:933:VAL:HG22	1:F:1021:GLU:HB2	1.89	0.54
1:B:932:LEU:HD22	1:B:935:ILE:HD11	1.90	0.54
1:B:313:ILE:HG23	1:B:316:ILE:HD12	1.90	0.54
1:E:877:ASN:ND2	1:E:895:THR:H	2.06	0.53
1:C:854:THR:HB	1:C:857:GLU:HB2	1.90	0.53
1:F:255:THR:HB	2:F:1119:IOD:I	2.78	0.53
1:D:645:THR:HG22	1:D:665:LEU:HD22	1.91	0.53
1:A:378:ALA:HA	1:A:401:SER:HB2	1.91	0.53
1:A:470:THR:HG23	1:A:471:VAL:HG23	1.91	0.53
1:D:933:VAL:HG22	1:D:1021:GLU:HB2	1.90	0.52
1:B:275:VAL:HG11	2:B:1117:IOD:I	2.78	0.52
1:C:945:ALA:HA	1:C:1017:ALA:HA	1.91	0.52
1:E:255:THR:HB	2:E:1116:IOD:I	2.80	0.52
1:C:800:VAL:HG22	1:C:820:GLY:HA3	1.92	0.51
1:E:956:ALA:HA	1:E:960:GLN:NE2	2.24	0.51
1:C:470:THR:HG22	4:C:1421:HOH:O	2.08	0.51
1:F:958:LEU:HB2	1:F:981:PHE:CE1	2.46	0.51
1:D:763:VAL:HG22	1:D:786:THR:HB	1.91	0.51
1:E:470:THR:HG23	1:E:471:VAL:HG23	1.91	0.51
1:C:703:VAL:HG11	1:C:729:THR:HG21	1.92	0.51
1:C:754:LEU:HD23	1:C:755:ALA:N	2.25	0.51
1:D:387:VAL:HG21	1:D:408:VAL:HG13	1.93	0.50
1:B:1018:PHE:CE1	1:B:1023:LEU:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:821:LEU:CD1	1:C:823:LEU:HB2	2.42	0.50
1:B:945:ALA:HA	1:B:1017:ALA:HA	1.94	0.49
1:F:946:PHE:CE1	1:F:978:TRP:HB3	2.47	0.49
1:B:930:LEU:HG	1:B:932:LEU:HD21	1.95	0.49
1:D:432:THR:HG23	2:D:1119:IOD:I	2.83	0.48
1:B:255:THR:HB	2:B:1117:IOD:I	2.83	0.48
1:F:416:THR:HB	1:F:444:ALA:HB2	1.95	0.48
1:B:950:VAL:HB	1:B:979:PHE:HB3	1.95	0.47
1:F:709:GLN:O	1:F:712:HIS:NE2	2.47	0.47
1:D:665:LEU:HD11	1:D:671:VAL:HG23	1.96	0.47
1:E:651:MET:HE3	1:E:658:VAL:HG22	1.96	0.47
1:B:639:SER:HA	1:B:657:THR:O	2.14	0.47
1:C:697:GLY:N	4:C:1222:HOH:O	2.37	0.47
1:A:558:GLU:HG3	1:A:562:ASP:HB3	1.95	0.47
1:C:522:GLY:O	1:C:550:THR:HA	2.14	0.47
1:E:929:LYS:HG2	1:E:1024:THR:HG23	1.96	0.47
1:C:264:THR:C	1:C:266:ASN:H	2.18	0.47
1:C:734:VAL:HG21	1:C:752:VAL:HG13	1.96	0.47
1:C:860:THR:HG23	4:C:1485:HOH:O	2.14	0.47
1:C:933:VAL:HG22	1:C:1021:GLU:HB2	1.96	0.47
1:B:522:GLY:O	1:B:550:THR:HA	2.15	0.47
1:F:971:SER:OG	1:F:993:ALA:HB2	2.14	0.47
1:E:950:VAL:HB	1:E:979:PHE:HB3	1.96	0.46
1:F:246:GLY:HA3	1:F:267:ASN:ND2	2.30	0.46
1:A:752:VAL:HB	1:A:781:LEU:HD23	1.96	0.46
1:E:998:VAL:HG12	1:E:1002:ASP:OD2	2.15	0.46
1:E:470:THR:HG22	4:E:1617:HOH:O	2.15	0.46
1:D:639:SER:HA	1:D:657:THR:O	2.16	0.46
1:C:821:LEU:HD13	1:C:823:LEU:HB2	1.98	0.46
1:F:522:GLY:O	1:F:550:THR:HA	2.16	0.46
1:A:992:SER:HA	2:A:1114:IOD:I	2.86	0.46
1:C:313:ILE:HG23	1:C:316:ILE:HD12	1.97	0.46
1:E:933:VAL:HG22	1:E:1021:GLU:HB2	1.97	0.46
1:C:300:GLN:O	1:C:323:SER:HA	2.16	0.45
1:B:969:ASP:OD2	1:B:993:ALA:HA	2.16	0.45
1:C:434:GLY:HA3	2:C:1110:IOD:I	2.86	0.45
1:F:558:GLU:HG3	1:F:562:ASP:HB3	1.98	0.45
1:F:988:VAL:HG13	1:F:997:PHE:HE1	1.81	0.45
1:E:957:THR:H	1:E:960:GLN:HE21	1.65	0.45
1:F:433:ALA:HB1	1:F:441:LEU:HD23	1.99	0.44
1:E:649:ILE:HG22	1:E:651:MET:HE1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:998:VAL:CG1	1:E:1001:ALA:HB3	2.47	0.44
1:E:752:VAL:HB	1:E:781:LEU:HD23	2.00	0.44
1:C:572:GLY:O	1:C:594:GLY:HA3	2.17	0.44
1:C:639:SER:HA	1:C:657:THR:O	2.17	0.44
1:D:789:ILE:O	1:D:815:VAL:HA	2.18	0.44
1:B:752:VAL:HB	1:B:781:LEU:HD23	1.98	0.44
1:A:300:GLN:O	1:A:323:SER:HA	2.17	0.44
1:A:255:THR:HB	2:A:1110:IOD:I	2.88	0.43
1:A:958:LEU:HB2	1:A:981:PHE:CE2	2.54	0.43
1:E:264:THR:C	1:E:266:ASN:H	2.21	0.43
1:A:567:THR:HG22	4:A:1201:HOH:O	2.18	0.43
1:D:541:LEU:HB2	1:D:565:PHE:CD2	2.54	0.43
1:E:804:THR:HA	1:E:824:THR:HB	2.00	0.43
1:A:709:GLN:HG2	4:A:1235:HOH:O	2.19	0.43
1:C:640:ILE:HG12	1:C:651:MET:HE3	2.01	0.43
1:E:503:PHE:CZ	1:E:522:GLY:HA3	2.53	0.43
1:F:600:ILE:HB	1:F:621:LEU:HD22	2.00	0.43
1:F:588:THR:HA	1:F:608:LEU:HA	2.00	0.43
1:F:967:ALA:O	4:F:1301:HOH:O	2.21	0.43
1:A:245:SER:HA	1:A:267:ASN:ND2	2.29	0.42
1:D:679:VAL:HG22	1:D:700:THR:HB	2.01	0.42
1:F:331:THR:HB	1:F:335:VAL:HG21	2.02	0.42
1:D:588:THR:HA	1:D:608:LEU:HA	2.02	0.42
1:E:946:PHE:HE2	1:E:977:LYS:HA	1.84	0.42
1:F:572:GLY:O	1:F:594:GLY:HA3	2.19	0.42
1:A:768:LEU:HB3	1:A:774:LEU:HD23	2.00	0.42
1:E:679:VAL:HG22	1:E:700:THR:HB	2.01	0.42
1:C:949:ALA:HB2	1:C:978:TRP:CZ2	2.55	0.42
1:E:958:LEU:HB2	1:E:981:PHE:CE2	2.55	0.42
1:F:841:GLY:HA2	2:F:1130:IOD:I	2.89	0.42
1:C:246:GLY:N	4:C:1253:HOH:O	2.53	0.42
1:D:257:GLY:HA2	1:E:275:VAL:HA	2.02	0.42
1:B:434:GLY:HA3	2:B:1116:IOD:I	2.90	0.42
1:B:946:PHE:HB3	1:B:1013:LEU:O	2.20	0.42
1:D:388:THR:OG1	1:D:389:SER:N	2.52	0.42
1:D:433:ALA:HB1	1:D:441:LEU:HD23	2.01	0.42
1:C:591:ASN:HB3	4:C:1414:HOH:O	2.19	0.41
1:D:912:ILE:HG23	1:D:1003:ALA:HB2	2.02	0.41
1:F:976:ALA:HA	1:F:988:VAL:O	2.20	0.41
1:B:470:THR:HG22	4:B:1878:HOH:O	2.20	0.41
1:D:522:GLY:O	1:D:550:THR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:433:ALA:HB1	1:E:441:LEU:HD23	2.02	0.41
1:E:450:GLY:O	1:E:484:SER:HB3	2.20	0.41
1:D:854:THR:HB	1:D:857:GLU:HB2	2.02	0.41
1:B:300:GLN:O	1:B:323:SER:HA	2.20	0.41
1:E:522:GLY:O	1:E:550:THR:HA	2.21	0.41
1:F:975:VAL:HG13	1:F:990:ASP:HB3	2.01	0.41
1:A:407:SER:HB3	2:A:1128:IOD:I	2.91	0.41
1:B:387:VAL:HG21	1:B:408:VAL:HG13	2.01	0.41
1:B:581:SER:HA	1:B:602:SER:O	2.20	0.41
1:F:854:THR:HB	1:F:857:GLU:HB2	2.02	0.41
1:F:950:VAL:HB	1:F:979:PHE:HB3	2.02	0.41
1:A:474:ARG:HH11	1:A:474:ARG:HD3	1.77	0.41
1:F:300:GLN:O	1:F:323:SER:HA	2.21	0.41
1:B:558:GLU:HG3	1:B:562:ASP:HB3	2.02	0.40
1:A:709:GLN:O	1:A:712:HIS:NE2	2.53	0.40
1:C:946:PHE:CZ	1:C:978:TRP:HB3	2.56	0.40
1:C:588:THR:HA	1:C:608:LEU:HA	2.03	0.40
1:D:659:THR:HA	1:D:681:VAL:HB	2.04	0.40
1:D:687:SER:HB2	1:D:689:PHE:CE2	2.57	0.40
1:C:734:VAL:O	1:C:754:LEU:HD23	2.20	0.40
1:F:686:GLY:HA2	1:F:711:SER:O	2.22	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	A	781/814 (96%)	759 (97%)	20 (3%)	2 (0%)	41	41
1	B	776/814 (95%)	750 (97%)	25 (3%)	1 (0%)	51	54
1	C	780/814 (96%)	752 (96%)	27 (4%)	1 (0%)	51	54
1	D	779/814 (96%)	755 (97%)	23 (3%)	1 (0%)	51	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	779/814 (96%)	753 (97%)	24 (3%)	2 (0%)	41	41
1	F	781/814 (96%)	754 (96%)	26 (3%)	1 (0%)	51	54
All	All	4676/4884 (96%)	4523 (97%)	145 (3%)	8 (0%)	47	49

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	265	ALA
1	A	246	GLY
1	A	502	SER
1	D	502	SER
1	E	502	SER
1	B	502	SER
1	C	502	SER
1	F	502	SER

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	530/554 (96%)	529 (100%)	1 (0%)	93	96
1	B	527/554 (95%)	526 (100%)	1 (0%)	93	96
1	C	529/554 (96%)	526 (99%)	3 (1%)	86	90
1	D	529/554 (96%)	526 (99%)	3 (1%)	86	90
1	E	528/554 (95%)	526 (100%)	2 (0%)	91	94
1	F	530/554 (96%)	529 (100%)	1 (0%)	93	96
All	All	3173/3324 (96%)	3162 (100%)	11 (0%)	92	95

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	946	PHE
1	B	946	PHE

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Mol	Chain	Res	Type
1	C	576	SER
1	C	862	ARG
1	C	946	PHE
1	D	537	THR
1	D	687	SER
1	D	946	PHE
1	E	573	SER
1	E	946	PHE
1	F	946	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	733	ASN
1	D	733	ASN
1	D	806	GLN
1	E	877	ASN
1	E	960	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 274 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	A	782/814 (96%)	-0.03	1 (0%) 95 96	15, 27, 38, 91	0
1	B	776/814 (95%)	0.07	8 (1%) 82 85	14, 30, 57, 100	0
1	C	781/814 (95%)	0.43	42 (5%) 25 31	18, 52, 72, 94	0
1	D	780/814 (95%)	0.16	13 (1%) 70 74	18, 45, 60, 86	0
1	E	781/814 (95%)	0.17	20 (2%) 56 61	19, 38, 68, 139	0
1	F	782/814 (96%)	0.12	27 (3%) 44 50	15, 34, 70, 146	0
All	All	4682/4884 (95%)	0.16	111 (2%) 59 64	14, 36, 65, 146	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	671	VAL	4.8
1	F	245	SER	4.0
1	B	946	PHE	3.9
1	E	469	ALA	3.8
1	F	948	ALA	3.8
1	E	246	GLY	3.7
1	E	940	ALA	3.7
1	E	998	VAL	3.6
1	A	245	SER	3.6
1	E	975	VAL	3.5
1	C	631	PHE	3.5
1	C	694	ALA	3.4
1	F	970	GLY	3.4
1	F	969	ASP	3.3
1	E	1000	GLY	3.3
1	C	666	GLY	3.3
1	C	698	PHE	3.3
1	F	437	VAL	3.3
1	D	469	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	946	PHE	3.1
1	C	696	GLY	3.1
1	B	1018	PHE	3.1
1	F	941	ILE	3.1
1	C	489	ALA	3.0
1	C	798	ALA	3.0
1	C	1018	PHE	3.0
1	C	944	GLY	2.9
1	F	975	VAL	2.9
1	F	1023	LEU	2.9
1	D	471	VAL	2.9
1	B	969	ASP	2.9
1	F	965	ALA	2.8
1	C	533	THR	2.8
1	F	968	GLY	2.8
1	D	650	VAL	2.8
1	F	1014	THR	2.8
1	B	1020	THR	2.7
1	C	490	THR	2.7
1	B	251	THR	2.7
1	C	471	VAL	2.7
1	E	946	PHE	2.7
1	B	945	ALA	2.7
1	F	942	ALA	2.7
1	F	1011	VAL	2.6
1	C	717	PHE	2.6
1	D	672	ASN	2.6
1	C	736	VAL	2.6
1	C	796	THR	2.6
1	C	800	VAL	2.5
1	C	469	ALA	2.5
1	C	667	ALA	2.5
1	E	995	ALA	2.5
1	C	264	THR	2.5
1	C	565	PHE	2.5
1	F	1026	ALA	2.5
1	C	760	THR	2.5
1	C	650	VAL	2.5
1	E	950	VAL	2.5
1	C	649	ILE	2.5
1	E	970	GLY	2.5
1	F	468	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	967	ALA	2.5
1	C	535	THR	2.4
1	E	796	THR	2.4
1	D	666	GLY	2.4
1	F	470	THR	2.4
1	E	471	VAL	2.4
1	C	246	GLY	2.4
1	E	1009	GLY	2.4
1	D	671	VAL	2.4
1	F	1018	PHE	2.3
1	C	486	ALA	2.3
1	C	1017	ALA	2.3
1	E	1018	PHE	2.3
1	C	691	ALA	2.3
1	F	796	THR	2.3
1	F	971	SER	2.3
1	C	695	PHE	2.3
1	E	942	ALA	2.3
1	D	468	GLY	2.3
1	F	972	GLY	2.2
1	F	1019	ALA	2.2
1	C	491	THR	2.2
1	D	934	GLY	2.2
1	E	969	ASP	2.2
1	C	487	ALA	2.2
1	F	943	ASP	2.2
1	C	946	PHE	2.2
1	E	467	ALA	2.2
1	C	1019	ALA	2.1
1	F	246	GLY	2.1
1	D	533	THR	2.1
1	E	997	PHE	2.1
1	F	997	PHE	2.1
1	C	468	GLY	2.1
1	C	927	GLY	2.1
1	C	488	SER	2.1
1	D	756	ASN	2.1
1	F	949	ALA	2.1
1	E	991	SER	2.1
1	E	1015	THR	2.1
1	B	943	ASP	2.0
1	C	612	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	1020	THR	2.0
1	C	665	LEU	2.0
1	C	942	ALA	2.0
1	B	975	VAL	2.0
1	C	764	PHE	2.0
1	D	470	THR	2.0
1	C	1011	VAL	2.0
1	D	669	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 carbohydrates 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	IOD	D	1122	1/1	0.78	0.07	130,130,130,130	1
2	IOD	B	1122	1/1	0.85	0.14	67,67,67,67	1
2	IOD	A	1129	1/1	0.90	0.09	84,84,84,84	1
2	IOD	B	1124	1/1	0.91	0.06	94,94,94,94	1
2	IOD	F	1130	1/1	0.92	0.09	93,93,93,93	1
2	IOD	E	1124	1/1	0.92	0.09	89,89,89,89	1
2	IOD	C	1118	1/1	0.92	0.06	89,89,89,89	1
3	SR	C	1141	1/1	0.92	0.11	25,25,25,25	1
2	IOD	F	1128	1/1	0.93	0.17	118,118,118,118	1
3	SR	F	1147	1/1	0.93	0.09	30,30,30,30	1
2	IOD	F	1129	1/1	0.93	0.07	69,69,69,69	1
2	IOD	E	1123	1/1	0.94	0.07	93,93,93,93	1
3	SR	C	1136	1/1	0.94	0.06	45,45,45,45	1
2	IOD	F	1127	1/1	0.94	0.07	59,59,59,59	1
2	IOD	C	1120	1/1	0.94	0.10	69,69,69,69	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SR	D	1142	1/1	0.94	0.10	70,70,70,70	1
2	IOD	A	1127	1/1	0.95	0.08	76,76,76,76	1
3	SR	C	1139	1/1	0.95	0.06	44,44,44,44	1
2	IOD	D	1113	1/1	0.95	0.06	58,58,58,58	1
3	SR	E	1126	1/1	0.95	0.08	38,38,38,38	0
3	SR	E	1143	1/1	0.95	0.06	36,36,36,36	1
2	IOD	E	1122	1/1	0.95	0.07	57,57,57,57	1
2	IOD	E	1119	1/1	0.95	0.09	72,72,72,72	1
2	IOD	D	1118	1/1	0.95	0.08	73,73,73,73	1
2	IOD	D	1121	1/1	0.95	0.09	101,101,101,101	1
3	SR	C	1129	1/1	0.95	0.07	45,45,45,45	1
2	IOD	A	1128	1/1	0.96	0.11	48,48,48,48	1
2	IOD	D	1117	1/1	0.96	0.05	62,62,62,62	1
3	SR	D	1141	1/1	0.96	0.09	32,32,32,32	1
2	IOD	C	1114	1/1	0.96	0.04	63,63,63,63	1
3	SR	E	1137	1/1	0.96	0.13	51,51,51,51	1
3	SR	E	1132	1/1	0.96	0.10	27,27,27,27	1
2	IOD	E	1120	1/1	0.96	0.09	63,63,63,63	1
3	SR	F	1146	1/1	0.96	0.06	73,73,73,73	0
3	SR	E	1142	1/1	0.97	0.11	34,34,34,34	1
2	IOD	C	1105	1/1	0.97	0.07	88,88,88,88	0
2	IOD	F	1115	1/1	0.97	0.05	50,50,50,50	1
2	IOD	B	1121	1/1	0.97	0.06	46,46,46,46	1
3	SR	E	1145	1/1	0.97	0.06	68,68,68,68	1
3	SR	C	1121	1/1	0.97	0.09	38,38,38,38	0
2	IOD	F	1118	1/1	0.97	0.06	51,51,51,51	1
3	SR	F	1149	1/1	0.97	0.08	35,35,35,35	1
2	IOD	A	1126	1/1	0.97	0.13	73,73,73,73	1
2	IOD	D	1119	1/1	0.97	0.11	64,64,64,64	1
3	SR	A	1149	1/1	0.97	0.04	47,47,47,47	1
2	IOD	F	1125	1/1	0.97	0.08	80,80,80,80	1
3	SR	B	1132	1/1	0.97	0.15	25,25,25,25	0
2	IOD	C	1112	1/1	0.97	0.06	54,54,54,54	1
2	IOD	A	1118	1/1	0.97	0.05	61,61,61,61	1
2	IOD	C	1116	1/1	0.97	0.08	72,72,72,72	1
3	SR	A	1146	1/1	0.97	0.10	26,26,26,26	1
3	SR	D	1128	1/1	0.97	0.03	50,50,50,50	0
2	IOD	A	1119	1/1	0.97	0.10	45,45,45,45	1
3	SR	C	1122	1/1	0.97	0.11	37,37,37,37	0
2	IOD	F	1121	1/1	0.97	0.14	61,61,61,61	1
3	SR	F	1144	1/1	0.97	0.06	68,68,68,68	0
3	SR	B	1143	1/1	0.97	0.10	32,32,32,32	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SR	E	1136	1/1	0.97	0.09	37,37,37,37	1
3	SR	C	1134	1/1	0.97	0.06	62,62,62,62	0
2	IOD	B	1112	1/1	0.97	0.08	88,88,88,88	0
3	SR	C	1130	1/1	0.97	0.04	55,55,55,55	0
2	IOD	E	1118	1/1	0.97	0.10	63,63,63,63	1
3	SR	E	1141	1/1	0.97	0.08	31,31,31,31	1
2	IOD	F	1119	1/1	0.97	0.10	45,45,45,45	1
3	SR	F	1150	1/1	0.98	0.10	32,32,32,32	1
3	SR	F	1137	1/1	0.98	0.08	41,41,41,41	1
3	SR	F	1148	1/1	0.98	0.07	28,28,28,28	1
3	SR	C	1125	1/1	0.98	0.05	53,53,53,53	0
3	SR	A	1140	1/1	0.98	0.07	39,39,39,39	0
2	IOD	C	1115	1/1	0.98	0.07	102,102,102,102	1
3	SR	F	1142	1/1	0.98	0.08	32,32,32,32	1
2	IOD	A	1123	1/1	0.98	0.15	69,69,69,69	1
2	IOD	C	1119	1/1	0.98	0.05	78,78,78,78	1
3	SR	B	1141	1/1	0.98	0.10	26,26,26,26	1
2	IOD	E	1115	1/1	0.98	0.10	54,54,54,54	1
2	IOD	C	1117	1/1	0.98	0.08	74,74,74,74	1
3	SR	B	1135	1/1	0.98	0.09	41,41,41,41	0
2	IOD	D	1120	1/1	0.98	0.06	73,73,73,73	1
2	IOD	E	1114	1/1	0.98	0.03	55,55,55,55	1
3	SR	B	1140	1/1	0.98	0.03	58,58,58,58	0
3	SR	E	1139	1/1	0.98	0.11	39,39,39,39	0
2	IOD	C	1111	1/1	0.98	0.09	59,59,59,59	1
3	SR	B	1129	1/1	0.98	0.09	37,37,37,37	0
3	SR	C	1133	1/1	0.98	0.02	60,60,60,60	0
3	SR	F	1152	1/1	0.98	0.10	36,36,36,36	1
3	SR	B	1136	1/1	0.98	0.04	55,55,55,55	0
2	IOD	D	1123	1/1	0.98	0.04	62,62,62,62	1
2	IOD	A	1125	1/1	0.98	0.12	57,57,57,57	1
3	SR	B	1144	1/1	0.98	0.11	27,27,27,27	1
2	IOD	B	1117	1/1	0.98	0.08	39,39,39,39	1
3	SR	C	1140	1/1	0.98	0.17	37,37,37,37	1
3	SR	E	1140	1/1	0.98	0.05	63,63,63,63	0
2	IOD	A	1122	1/1	0.98	0.06	45,45,45,45	1
2	IOD	D	1115	1/1	0.98	0.04	67,67,67,67	1
2	IOD	B	1114	1/1	0.98	0.07	69,69,69,69	1
3	SR	D	1126	1/1	0.98	0.04	48,48,48,48	0
3	SR	E	1127	1/1	0.98	0.10	42,42,42,42	1
2	IOD	E	1121	1/1	0.98	0.08	73,73,73,73	1
2	IOD	C	1110	1/1	0.98	0.11	64,64,64,64	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SR	D	1124	1/1	0.98	0.10	32,32,32,32	0
3	SR	E	1133	1/1	0.98	0.09	35,35,35,35	1
2	IOD	E	1109	1/1	0.98	0.09	94,94,94,94	0
3	SR	B	1142	1/1	0.98	0.09	32,32,32,32	1
3	SR	D	1137	1/1	0.98	0.11	29,29,29,29	1
2	IOD	E	1106	1/1	0.98	0.07	52,52,52,52	1
3	SR	F	1136	1/1	0.98	0.12	25,25,25,25	1
2	IOD	F	1110	1/1	0.98	0.13	61,61,61,61	1
2	IOD	F	1122	1/1	0.98	0.06	63,63,63,63	1
3	SR	D	1138	1/1	0.98	0.04	57,57,57,57	0
2	IOD	E	1108	1/1	0.98	0.07	95,95,95,95	0
3	SR	F	1145	1/1	0.98	0.03	66,66,66,66	0
3	SR	C	1132	1/1	0.98	0.07	39,39,39,39	1
3	SR	C	1131	1/1	0.99	0.03	53,53,53,53	0
3	SR	B	1138	1/1	0.99	0.11	36,36,36,36	0
3	SR	C	1123	1/1	0.99	0.05	48,48,48,48	0
3	SR	D	1132	1/1	0.99	0.10	31,31,31,31	0
2	IOD	E	1116	1/1	0.99	0.07	60,60,60,60	1
3	SR	D	1133	1/1	0.99	0.09	35,35,35,35	1
2	IOD	D	1116	1/1	0.99	0.13	40,40,40,40	1
2	IOD	F	1101	1/1	0.99	0.12	54,54,54,54	1
3	SR	B	1134	1/1	0.99	0.09	31,31,31,31	0
3	SR	B	1139	1/1	0.99	0.09	32,32,32,32	1
3	SR	E	1135	1/1	0.99	0.07	39,39,39,39	0
3	SR	A	1143	1/1	0.99	0.12	31,31,31,31	0
3	SR	E	1125	1/1	0.99	0.10	39,39,39,39	0
2	IOD	D	1111	1/1	0.99	0.08	50,50,50,50	1
2	IOD	F	1126	1/1	0.99	0.06	53,53,53,53	1
2	IOD	F	1124	1/1	0.99	0.14	38,38,38,38	0
2	IOD	A	1104	1/1	0.99	0.12	42,42,42,42	1
2	IOD	F	1112	1/1	0.99	0.12	40,40,40,40	1
3	SR	A	1147	1/1	0.99	0.10	28,28,28,28	1
2	IOD	F	1108	1/1	0.99	0.10	37,37,37,37	1
2	IOD	C	1102	1/1	0.99	0.09	53,53,53,53	1
2	IOD	D	1108	1/1	0.99	0.06	49,49,49,49	1
3	SR	B	1126	1/1	0.99	0.17	28,28,28,28	0
2	IOD	E	1103	1/1	0.99	0.11	50,50,50,50	1
3	SR	B	1131	1/1	0.99	0.12	27,27,27,27	1
2	IOD	A	1117	1/1	0.99	0.12	35,35,35,35	1
3	SR	F	1132	1/1	0.99	0.12	30,30,30,30	0
3	SR	E	1130	1/1	0.99	0.11	27,27,27,27	0
2	IOD	E	1117	1/1	0.99	0.05	51,51,51,51	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IOD	F	1111	1/1	0.99	0.13	33,33,33,33	1
3	SR	A	1137	1/1	0.99	0.10	34,34,34,34	0
3	SR	C	1137	1/1	0.99	0.03	48,48,48,48	0
2	IOD	F	1120	1/1	0.99	0.07	48,48,48,48	1
2	IOD	A	1102	1/1	0.99	0.12	45,45,45,45	0
2	IOD	F	1116	1/1	0.99	0.06	45,45,45,45	1
2	IOD	C	1107	1/1	0.99	0.09	55,55,55,55	1
3	SR	A	1138	1/1	0.99	0.14	28,28,28,28	0
2	IOD	F	1123	1/1	0.99	0.03	57,57,57,57	1
3	SR	E	1138	1/1	0.99	0.04	62,62,62,62	0
2	IOD	B	1110	1/1	0.99	0.11	41,41,41,41	1
3	SR	F	1141	1/1	0.99	0.09	36,36,36,36	1
2	IOD	E	1104	1/1	0.99	0.13	35,35,35,35	1
2	IOD	A	1110	1/1	0.99	0.08	39,39,39,39	1
2	IOD	E	1113	1/1	0.99	0.07	91,91,91,91	0
2	IOD	A	1112	1/1	0.99	0.09	46,46,46,46	1
3	SR	D	1139	1/1	0.99	0.06	43,43,43,43	0
3	SR	B	1128	1/1	0.99	0.07	40,40,40,40	0
3	SR	C	1126	1/1	0.99	0.08	43,43,43,43	1
3	SR	F	1143	1/1	0.99	0.12	37,37,37,37	0
3	SR	E	1131	1/1	0.99	0.10	36,36,36,36	0
3	SR	E	1129	1/1	0.99	0.08	37,37,37,37	1
2	IOD	F	1103	1/1	0.99	0.16	36,36,36,36	0
3	SR	F	1133	1/1	0.99	0.09	37,37,37,37	0
2	IOD	D	1105	1/1	0.99	0.05	55,55,55,55	1
3	SR	F	1140	1/1	0.99	0.10	36,36,36,36	0
3	SR	F	1131	1/1	0.99	0.13	30,30,30,30	0
2	IOD	B	1120	1/1	0.99	0.06	55,55,55,55	1
2	IOD	D	1112	1/1	0.99	0.06	49,49,49,49	1
3	SR	B	1130	1/1	0.99	0.09	43,43,43,43	0
3	SR	C	1124	1/1	0.99	0.06	43,43,43,43	1
2	IOD	F	1107	1/1	0.99	0.06	51,51,51,51	1
2	IOD	B	1106	1/1	0.99	0.12	37,37,37,37	1
3	SR	E	1134	1/1	0.99	0.08	37,37,37,37	1
3	SR	C	1138	1/1	0.99	0.06	36,36,36,36	1
2	IOD	F	1105	1/1	0.99	0.14	39,39,39,39	1
2	IOD	E	1105	1/1	0.99	0.09	67,67,67,67	0
2	IOD	E	1107	1/1	0.99	0.10	42,42,42,42	1
3	SR	D	1140	1/1	0.99	0.06	33,33,33,33	1
3	SR	A	1148	1/1	0.99	0.13	59,59,59,59	1
3	SR	B	1127	1/1	0.99	0.15	26,26,26,26	0
2	IOD	E	1111	1/1	0.99	0.10	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SR	D	1136	1/1	0.99	0.04	57,57,57,57	0
3	SR	A	1134	1/1	0.99	0.05	40,40,40,40	0
3	SR	C	1127	1/1	0.99	0.06	43,43,43,43	1
2	IOD	B	1105	1/1	0.99	0.10	51,51,51,51	1
3	SR	E	1144	1/1	0.99	0.12	29,29,29,29	1
3	SR	A	1136	1/1	0.99	0.10	35,35,35,35	0
2	IOD	A	1121	1/1	0.99	0.11	50,50,50,50	1
3	SR	A	1139	1/1	0.99	0.12	34,34,34,34	0
3	SR	C	1135	1/1	0.99	0.07	39,39,39,39	1
2	IOD	B	1119	1/1	0.99	0.09	68,68,68,68	1
2	IOD	D	1114	1/1	0.99	0.06	61,61,61,61	1
2	IOD	A	1115	1/1	0.99	0.06	42,42,42,42	1
3	SR	F	1134	1/1	0.99	0.14	25,25,25,25	0
2	IOD	A	1109	1/1	0.99	0.13	38,38,38,38	1
2	IOD	B	1109	1/1	0.99	0.12	41,41,41,41	1
3	SR	A	1142	1/1	0.99	0.10	29,29,29,29	1
3	SR	D	1134	1/1	0.99	0.08	45,45,45,45	0
3	SR	A	1135	1/1	0.99	0.06	38,38,38,38	0
3	SR	A	1130	1/1	0.99	0.13	31,31,31,31	0
3	SR	F	1153	1/1	0.99	0.08	34,34,34,34	1
3	SR	A	1131	1/1	0.99	0.09	35,35,35,35	0
3	SR	F	1135	1/1	0.99	0.09	36,36,36,36	0
3	SR	B	1125	1/1	0.99	0.09	32,32,32,32	0
2	IOD	E	1110	1/1	0.99	0.09	41,41,41,41	1
3	SR	F	1151	1/1	0.99	0.09	24,24,24,24	1
3	SR	D	1125	1/1	0.99	0.13	29,29,29,29	0
2	IOD	B	1115	1/1	0.99	0.10	39,39,39,39	1
3	SR	F	1139	1/1	0.99	0.09	34,34,34,34	1
2	IOD	B	1118	1/1	0.99	0.06	54,54,54,54	1
2	IOD	A	1113	1/1	0.99	0.13	40,40,40,40	1
2	IOD	D	1110	1/1	0.99	0.08	53,53,53,53	1
2	IOD	C	1108	1/1	0.99	0.07	70,70,70,70	1
3	SR	E	1128	1/1	0.99	0.08	41,41,41,41	0
2	IOD	E	1112	1/1	0.99	0.07	45,45,45,45	1
3	SR	D	1130	1/1	0.99	0.06	45,45,45,45	0
3	SR	D	1135	1/1	0.99	0.02	51,51,51,51	0
2	IOD	B	1111	1/1	0.99	0.10	48,48,48,48	1
3	SR	D	1127	1/1	0.99	0.10	40,40,40,40	1
2	IOD	D	1106	1/1	0.99	0.07	50,50,50,50	1
2	IOD	C	1113	1/1	0.99	0.06	60,60,60,60	1
2	IOD	F	1106	1/1	0.99	0.14	37,37,37,37	1
2	IOD	B	1123	1/1	0.99	0.06	69,69,69,69	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IOD	A	1124	1/1	0.99	0.07	57,57,57,57	1
3	SR	B	1137	1/1	0.99	0.04	53,53,53,53	0
2	IOD	A	1116	1/1	0.99	0.12	34,34,34,34	1
3	SR	A	1141	1/1	0.99	0.11	32,32,32,32	0
2	IOD	B	1102	1/1	1.00	0.11	44,44,44,44	0
3	SR	C	1128	1/1	1.00	0.12	31,31,31,31	0
2	IOD	D	1102	1/1	1.00	0.11	54,54,54,54	0
3	SR	A	1144	1/1	1.00	0.12	32,32,32,32	0
2	IOD	A	1114	1/1	1.00	0.08	49,49,49,49	1
2	IOD	E	1102	1/1	1.00	0.16	45,45,45,45	0
2	IOD	A	1103	1/1	1.00	0.13	42,42,42,42	1
2	IOD	C	1106	1/1	1.00	0.10	50,50,50,50	1
3	SR	B	1133	1/1	1.00	0.03	45,45,45,45	0
2	IOD	D	1101	1/1	1.00	0.11	46,46,46,46	1
2	IOD	C	1104	1/1	1.00	0.14	47,47,47,47	1
2	IOD	A	1120	1/1	1.00	0.07	44,44,44,44	1
2	IOD	A	1101	1/1	1.00	0.12	42,42,42,42	0
3	SR	A	1145	1/1	1.00	0.10	36,36,36,36	0
2	IOD	D	1109	1/1	1.00	0.08	37,37,37,37	1
2	IOD	B	1101	1/1	1.00	0.13	42,42,42,42	0
2	IOD	B	1113	1/1	1.00	0.07	37,37,37,37	1
2	IOD	B	1103	1/1	1.00	0.12	35,35,35,35	1
2	IOD	C	1101	1/1	1.00	0.07	57,57,57,57	0
2	IOD	D	1107	1/1	1.00	0.09	58,58,58,58	1
2	IOD	D	1103	1/1	1.00	0.08	46,46,46,46	1
2	IOD	F	1117	1/1	1.00	0.07	50,50,50,50	1
2	IOD	C	1109	1/1	1.00	0.10	36,36,36,36	1
3	SR	F	1138	1/1	1.00	0.10	37,37,37,37	0
3	SR	A	1132	1/1	1.00	0.08	36,36,36,36	0
2	IOD	B	1104	1/1	1.00	0.12	42,42,42,42	1
2	IOD	A	1111	1/1	1.00	0.08	38,38,38,38	1
3	SR	D	1129	1/1	1.00	0.03	48,48,48,48	0
2	IOD	F	1104	1/1	1.00	0.12	41,41,41,41	1
2	IOD	A	1107	1/1	1.00	0.11	39,39,39,39	1
2	IOD	F	1114	1/1	1.00	0.10	44,44,44,44	1
2	IOD	D	1104	1/1	1.00	0.11	48,48,48,48	1
2	IOD	A	1106	1/1	1.00	0.10	39,39,39,39	1
2	IOD	F	1113	1/1	1.00	0.08	45,45,45,45	1
2	IOD	A	1105	1/1	1.00	0.09	46,46,46,46	1
3	SR	D	1131	1/1	1.00	0.06	36,36,36,36	1
2	IOD	F	1102	1/1	1.00	0.11	47,47,47,47	0
2	IOD	E	1101	1/1	1.00	0.11	47,47,47,47	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IOD	B	1108	1/1	1.00	0.13	41,41,41,41	1
2	IOD	B	1116	1/1	1.00	0.07	40,40,40,40	1
2	IOD	B	1107	1/1	1.00	0.12	38,38,38,38	1
2	IOD	C	1103	1/1	1.00	0.08	53,53,53,53	1
2	IOD	A	1108	1/1	1.00	0.10	43,43,43,43	1
2	IOD	F	1109	1/1	1.00	0.11	40,40,40,40	1
3	SR	A	1133	1/1	1.00	0.10	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.