



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2017 – 11:56 AM EDT

PDB ID : 3H02
Title : 2.15 Angstrom Resolution Crystal Structure of Naphthoate Synthase from *Salmonella typhimurium*.
Authors : Minasov, G.; Wawrzak, Z.; Skarina, T.; Onopriyenko, O.; Peterson, S.N.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID); Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : unknown
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

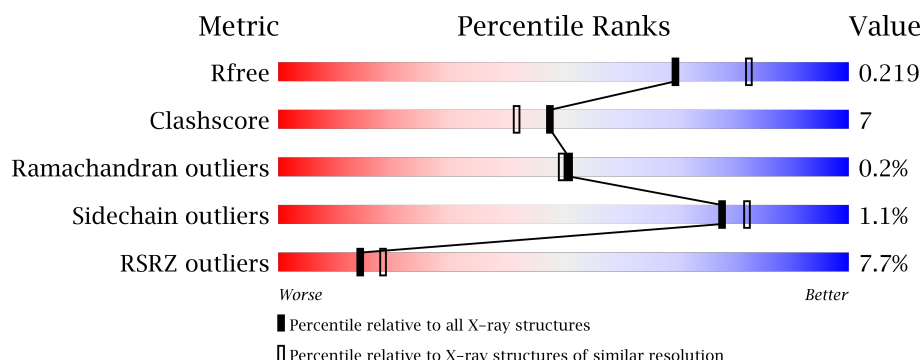
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	100719	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	288	<div> <div>5%</div> <div>80% 13% 8%</div> </div>
1	B	288	<div> <div>8%</div> <div>79% 12% 9%</div> </div>
1	C	288	<div> <div>12%</div> <div>78% 12% 9%</div> </div>
1	D	288	<div> <div>7%</div> <div>79% 13% 8%</div> </div>
1	E	288	<div> <div>7%</div> <div>81% 10% 8%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	288	

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	SO4	A	286	-	-	X	X
2	SO4	F	286	-	-	X	X
3	BCT	A	287	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13009 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 Naphthoate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	Se	0	5	0
			2111	1318	378	396	8	11			
1	B	262	Total	C	N	O	S	Se	0	4	0
			2071	1294	372	386	8	11			
1	C	262	Total	C	N	O	S	Se	0	5	0
			2075	1297	369	390	8	11			
1	D	264	Total	C	N	O	S	Se	0	4	0
			2081	1302	367	393	8	11			
1	E	264	Total	C	N	O	S	Se	0	4	0
			2088	1306	368	395	8	11			
1	F	239	Total	C	N	O	S	Se	0	6	0
			1893	1186	332	356	8	11			

There are 18 discrepancies between the modelled and reference sequences:

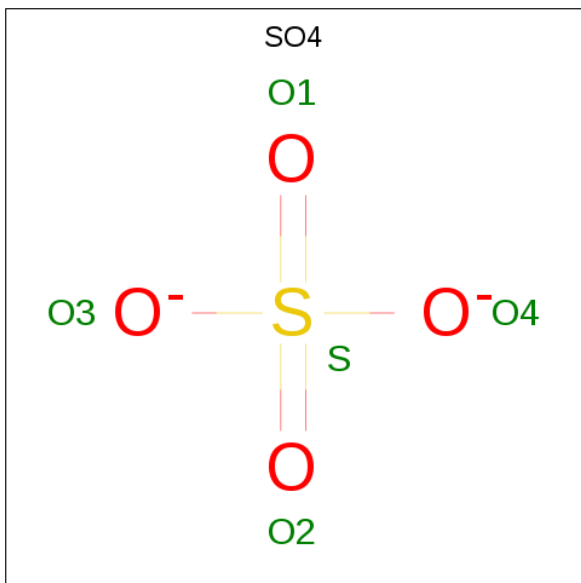
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
A	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
A	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
B	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
B	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
B	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
C	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
C	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
C	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
D	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
D	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
D	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
E	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
E	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56
E	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56
F	-2	SER	-	EXPRESSION TAG	UNP Q7CQ56
F	-1	ASN	-	EXPRESSION TAG	UNP Q7CQ56

Continued on next page...

Continued from previous page...

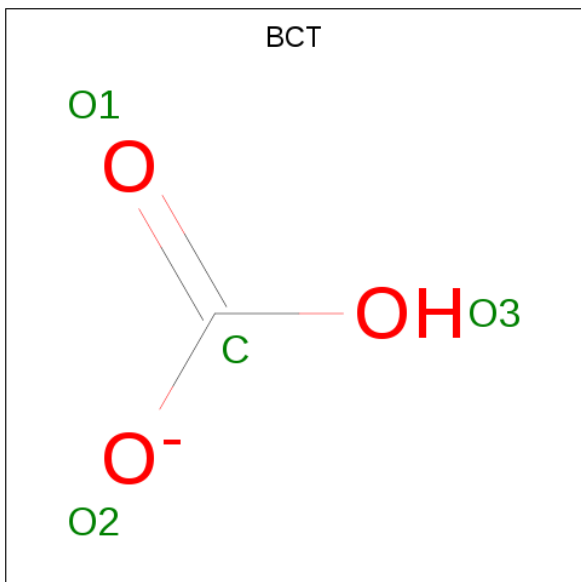
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	EXPRESSION TAG	UNP Q7CQ56

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 1 3	0	0
3	B	1	Total C O 4 1 3	0	0
3	C	1	Total C O 4 1 3	0	0
3	D	1	Total C O 4 1 3	0	0
3	E	1	Total C O 4 1 3	0	0
3	F	1	Total C O 4 1 3	0	0
3	F	1	Total C O 4 1 3	0	0

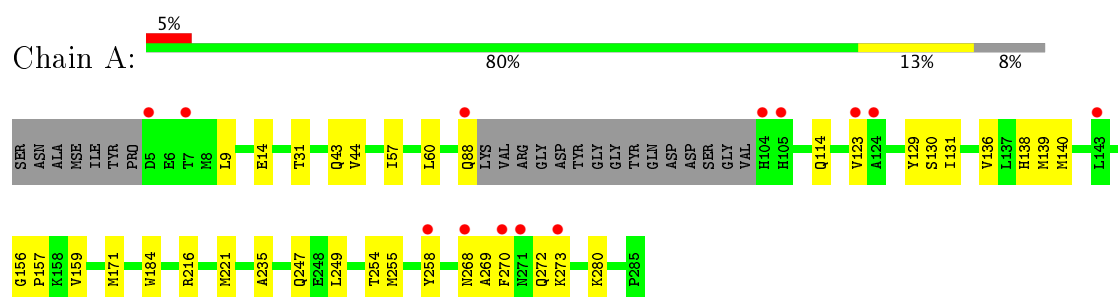
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	115	Total O 117 117	0	2
4	B	109	Total O 115 115	0	9
4	C	93	Total O 97 97	0	5
4	D	94	Total O 97 97	0	4
4	E	101	Total O 108 108	0	9
4	F	114	Total O 118 118	0	9

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.

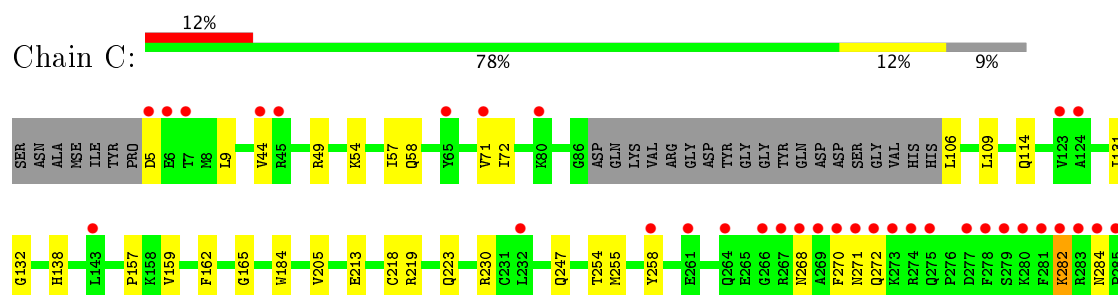
• Molecule 1: Naphthoate synthase



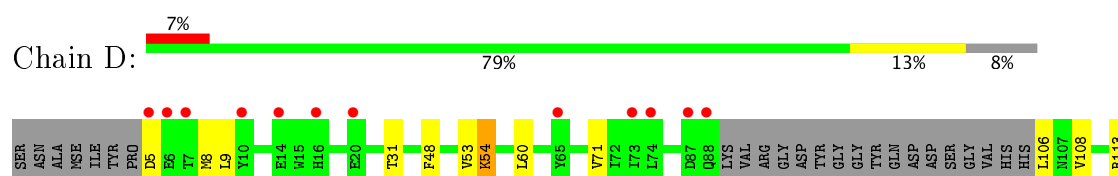
• Molecule 1: Naphthoate synthase

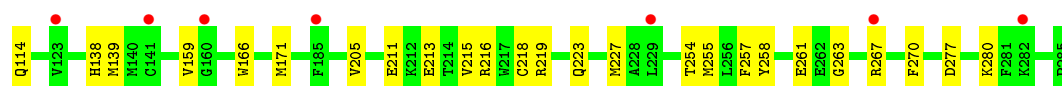


• Molecule 1: Naphthoate synthase

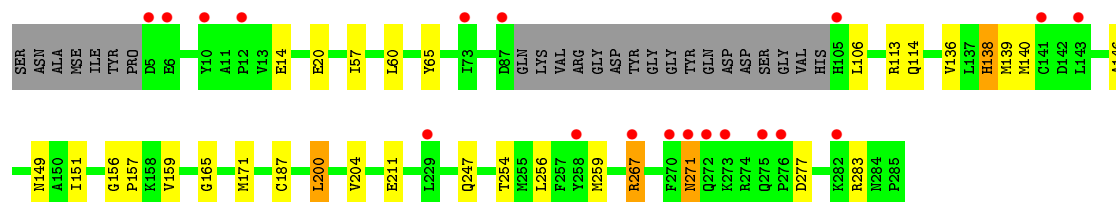
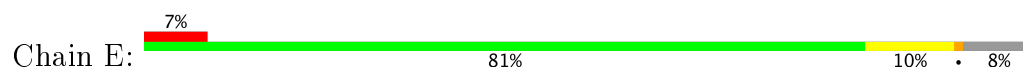


• Molecule 1: Naphthoate synthase

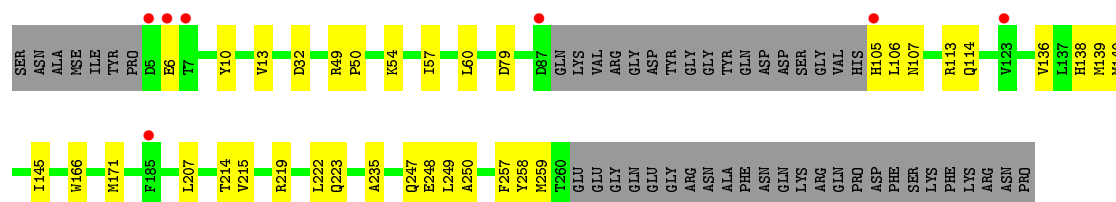




• Molecule 1: Naphthoate synthase



• Molecule 1: Naphthoate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.90Å 132.82Å 151.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.15 29.60 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.83-2.15) 98.6 (29.60-2.15)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.61 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0051	Depositor
R, R_{free}	0.169 , 0.215 0.177 , 0.219	Depositor DCC
R_{free} test set	4153 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13009	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, SO4

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	0.51	0/2139	0.66	0/2867
1	B	0.54	0/2099	0.70	0/2812
1	C	0.48	0/2101	0.65	0/2815
1	D	0.49	0/2107	0.67	0/2825
1	E	0.51	0/2115	0.66	0/2833
1	F	0.54	0/1915	0.68	0/2569
All	All	0.51	0/12476	0.67	0/16721

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	2111	0	2062	26	0
1	B	2071	0	2027	35	0
1	C	2075	0	2034	30	0
1	D	2081	0	2038	30	0
1	E	2088	0	2032	35	0
1	F	1893	0	1858	30	0
2	A	5	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	5	0	0	2	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	8	0	0	1	0
4	A	117	0	0	4	0
4	B	115	0	0	4	0
4	C	97	0	0	2	0
4	D	97	0	0	2	0
4	E	108	0	0	1	0
4	F	118	0	0	5	0
All	All	13009	0	12051	172	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 7.

All (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:VAL:O	1:C:44:VAL:HG12	1.65	0.96
1:C:268:ASN:O	1:C:272:GLN:HG3	1.69	0.92
1:C:5:ASP:O	1:C:9:LEU:HD13	1.71	0.89
1:F:13:VAL:HG23	4:F:407:HOH:O	1.72	0.89
1:D:205:VAL:HG11	1:D:213:GLU:HG2	1.55	0.88
2:F:286:SO4:S	4:F:583:HOH:O	2.33	0.87
1:D:159[A]:VAL:O	1:D:159[A]:VAL:HG12	1.71	0.87
1:E:267:ARG:HH11	1:E:267:ARG:HG3	1.40	0.86
4:B:322:HOH:O	1:F:250:ALA:HB2	1.74	0.86
1:E:256:LEU:HA	1:E:259:MSE:HE2	1.55	0.86
1:A:159[A]:VAL:O	1:A:159[A]:VAL:HG12	1.76	0.85
2:A:286:SO4:S	4:A:589:HOH:O	2.34	0.85
1:C:106:LEU:O	1:C:106:LEU:HD12	1.84	0.78
1:A:130:SER:C	1:A:131:ILE:HD12	2.03	0.78
1:A:88:GLN:HG2	1:D:270:PHE:CE2	2.20	0.77
1:F:60:LEU:HD23	1:F:114:GLN:HG2	1.67	0.77
1:A:268:ASN:O	1:A:272:GLN:HG3	1.85	0.76
1:E:267:ARG:CG	1:E:267:ARG:HH11	1.98	0.76
1:C:159:VAL:HG12	1:C:159:VAL:O	1.85	0.75
1:E:271:ASN:HD22	1:E:271:ASN:C	1.92	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:VAL:O	1:C:44:VAL:CG1	2.38	0.72
1:B:13:VAL:HG11	1:B:215:VAL:HG11	1.71	0.72
1:B:65:TYR:HE2	1:F:105:HIS:HE2	1.39	0.71
1:B:113[A]:ARG:HD3	1:B:166:TRP:HH2	1.53	0.71
1:B:105:HIS:CD2	1:B:107:ASN:HB3	2.25	0.70
1:B:113[A]:ARG:CD	1:B:166:TRP:HH2	2.04	0.70
1:E:57:ILE:HG23	1:E:114:GLN:OE1	1.92	0.70
1:E:256:LEU:HD23	1:E:259:MSE:CE	2.21	0.70
1:A:270:PHE:O	1:A:273:LYS:HG3	1.92	0.70
1:B:113[A]:ARG:NE	1:B:166:TRP:HH2	1.91	0.68
1:E:149:ASN:O	1:E:151:ILE:HD12	1.93	0.68
1:E:271:ASN:C	1:E:271:ASN:ND2	2.47	0.67
1:A:57:ILE:HG23	1:A:114:GLN:OE1	1.95	0.66
1:D:227:MSE:HE1	1:D:255:MSE:HE1	1.76	0.66
1:A:60:LEU:HD23	1:A:114:GLN:HG2	1.76	0.66
1:B:219:ARG:O	1:B:223:GLN:HG2	1.94	0.66
1:A:129:TYR:HB3	1:A:131:ILE:HD13	1.78	0.65
1:B:13:VAL:HG12	1:B:219:ARG:NH1	2.13	0.64
1:D:227:MSE:HE1	1:D:255:MSE:CE	2.28	0.64
1:B:13:VAL:CG1	1:B:215:VAL:HG11	2.28	0.64
1:C:205:VAL:HG11	1:C:213:GLU:HG3	1.81	0.62
1:D:48:PHE:CE1	1:D:108[A]:VAL:HG21	2.34	0.62
1:D:159[A]:VAL:O	1:D:159[A]:VAL:CG1	2.42	0.62
1:A:159[A]:VAL:O	1:A:159[A]:VAL:CG1	2.48	0.61
1:B:113[A]:ARG:NE	1:B:166:TRP:CH2	2.68	0.61
1:A:14:GLU:OE2	1:A:31:THR:HG21	2.01	0.60
1:D:53:VAL:HG21	1:D:108[A]:VAL:HG22	1.81	0.60
1:E:159:VAL:HG12	1:E:159:VAL:O	2.02	0.60
1:A:249[A]:LEU:HD21	4:B:322:HOH:O	2.03	0.59
1:E:271:ASN:ND2	1:E:271:ASN:O	2.32	0.59
1:C:106:LEU:O	1:C:106:LEU:CD1	2.50	0.59
1:E:256:LEU:HA	1:E:259:MSE:CE	2.32	0.59
1:E:256:LEU:HD23	1:E:259:MSE:HE1	1.83	0.59
1:E:149:ASN:O	1:E:151:ILE:CD1	2.51	0.58
1:F:13:VAL:CG2	4:F:407:HOH:O	2.40	0.58
1:F:6:GLU:HG3	1:F:10:TYR:CD2	2.38	0.58
1:F:79:ASP:HB3	1:F:207:LEU:HD21	1.85	0.58
1:B:205:VAL:HG11	1:B:213:GLU:HG2	1.86	0.58
1:A:139:MSE:HE1	1:A:171:MSE:HE3	1.85	0.57
1:B:113[A]:ARG:HD3	1:B:166:TRP:CH2	2.38	0.57
1:C:106:LEU:HD13	1:C:109:LEU:HD22	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:THR:HG22	1:C:258:TYR:CE2	2.40	0.56
1:B:260:THR:HG21	1:E:259:MSE:HE3	1.86	0.55
1:D:54:LYS:HA	1:D:54:LYS:HE2	1.88	0.55
1:C:57:ILE:HG23	1:C:114:GLN:OE1	2.05	0.55
1:A:235:ALA:HA	1:A:249[B]:LEU:HD21	1.88	0.55
1:E:267:ARG:NH1	1:E:267:ARG:HG3	2.17	0.54
1:F:6:GLU:HG3	1:F:10:TYR:HD2	1.72	0.53
1:D:71[A]:VAL:HG11	1:D:218:CYS:HB3	1.91	0.53
1:C:5:ASP:C	1:C:9:LEU:HD13	2.28	0.53
1:E:151:ILE:N	1:E:151:ILE:HD12	2.24	0.53
1:B:113[A]:ARG:HD2	1:F:113[A]:ARG:HH21	1.73	0.52
1:E:211[A]:GLU:CD	1:E:211[A]:GLU:H	2.12	0.52
1:F:257:PHE:C	1:F:259:MSE:H	2.12	0.52
1:A:247:GLN:OE1	1:D:113:ARG:NH1	2.40	0.52
1:B:113[B]:ARG:NH2	4:B:494:HOH:O	2.43	0.51
1:B:160:GLY:O	1:F:257:PHE:CZ	2.64	0.51
1:D:106:LEU:HD12	1:D:106:LEU:N	2.26	0.51
1:D:139:MSE:HE1	1:D:171:MSE:HE3	1.93	0.51
1:B:65:TYR:HE2	1:F:105:HIS:NE2	2.07	0.50
1:C:71[B]:VAL:HG21	1:C:218:CYS:HB3	1.92	0.50
1:F:235:ALA:HA	1:F:249[B]:LEU:HD21	1.93	0.50
1:B:113[B]:ARG:O	1:B:116:ARG:HB3	2.11	0.50
1:C:72:ILE:N	1:C:72:ILE:HD12	2.26	0.50
1:B:159:VAL:HG12	1:B:159:VAL:O	2.12	0.50
1:E:283:ARG:NH1	4:E:413:HOH:O	2.45	0.50
1:B:139:MSE:HE1	1:B:171:MSE:HE3	1.94	0.49
1:F:60:LEU:CD2	1:F:114:GLN:HG2	2.39	0.49
1:B:257:PHE:O	1:B:263:GLY:HA3	2.13	0.49
1:D:267:ARG:C	1:D:267:ARG:HD2	2.32	0.49
1:A:269:ALA:O	1:A:273:LYS:N	2.45	0.49
1:A:255:MSE:HG2	1:D:106:LEU:HD22	1.95	0.49
3:F:287:BCT:C	4:F:630:HOH:O	2.61	0.48
1:E:139:MSE:HE1	1:E:171:MSE:HE3	1.95	0.48
1:C:282:LYS:H	1:C:282:LYS:HD2	1.78	0.48
1:A:249[A]:LEU:HD23	1:F:249[A]:LEU:HD23	1.96	0.48
2:A:286:SO4:O3	4:A:589:HOH:O	2.20	0.48
1:D:5:ASP:HB3	1:D:8:MSE:HE3	1.96	0.48
1:F:113[A]:ARG:HG2	1:F:166:TRP:CH2	2.49	0.48
1:D:113:ARG:HG2	1:D:166:TRP:CH2	2.49	0.48
1:E:138:HIS:CE1	1:E:200:LEU:HD22	2.49	0.48
1:B:163[B]:ASP:OD1	1:B:163[B]:ASP:C	2.51	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:PRO:HD2	1:E:187:CYS:SG	2.54	0.47
1:A:9:LEU:HB3	1:A:216:ARG:HG3	1.96	0.47
1:B:26:ARG:HB2	1:B:38:THR:HB	1.96	0.47
1:A:136:VAL:O	1:A:140:MSE:HG2	2.13	0.47
1:D:54:LYS:HE3	4:D:477:HOH:O	2.14	0.47
1:F:13:VAL:HG22	1:F:215:VAL:HG11	1.96	0.47
1:D:261:GLU:HG2	4:D:398:HOH:O	2.14	0.47
1:A:131:ILE:HD12	1:A:131:ILE:N	2.29	0.47
1:C:58:GLN:HG3	4:C:378:HOH:O	2.14	0.47
1:F:145:ILE:HD12	1:F:214:THR:HA	1.96	0.46
4:C:297:HOH:O	1:E:113:ARG:HD3	2.15	0.46
1:B:254:THR:HG22	1:B:258:TYR:CE1	2.50	0.46
1:C:159:VAL:CG1	1:C:159:VAL:O	2.57	0.46
1:D:9:LEU:HB3	1:D:216:ARG:HG3	1.98	0.46
1:B:70:GLY:HA2	1:E:283:ARG:HD3	1.96	0.46
1:B:160:GLY:O	1:F:257:PHE:CE2	2.68	0.46
1:F:106:LEU:HD12	1:F:106:LEU:N	2.29	0.46
1:C:131:ILE:HG22	1:C:132:GLY:N	2.30	0.46
1:A:43:GLN:HG2	1:A:44:VAL:HG13	1.97	0.46
4:A:394:HOH:O	1:D:113:ARG:HD3	2.16	0.45
1:C:284:ASN:HD22	1:D:255:MSE:HE3	1.80	0.45
1:B:113[B]:ARG:HH22	1:F:248:GLU:HG2	1.81	0.45
1:C:230:ARG:NH2	1:C:255:MSE:HE1	2.32	0.45
1:E:14:GLU:O	1:E:14:GLU:HG3	2.16	0.45
1:B:165:GLY:HA3	1:F:247:GLN:HA	1.99	0.45
1:C:247:GLN:HA	1:E:165:GLY:HA3	1.98	0.45
1:D:211:GLU:O	1:D:215:VAL:HG23	2.18	0.44
1:A:157:PRO:HG2	1:A:184:TRP:O	2.17	0.44
1:C:157:PRO:HG2	1:C:184:TRP:O	2.18	0.44
1:F:219:ARG:O	1:F:223:GLN:HG2	2.18	0.43
1:A:254:THR:O	1:A:258:TYR:HD2	2.02	0.43
1:B:26:ARG:HG2	4:B:444:HOH:O	2.18	0.43
1:C:219:ARG:O	1:C:223[A]:GLN:HG2	2.19	0.43
1:C:282:LYS:N	1:C:282:LYS:HD2	2.34	0.43
1:A:123:VAL:CG2	1:A:221:MSE:HE1	2.49	0.43
1:F:32:ASP:O	1:F:222:LEU:HD13	2.19	0.43
1:D:254:THR:HG22	1:D:258:TYR:CE2	2.54	0.43
1:B:147:ALA:HB2	1:B:210:LEU:HD22	2.00	0.43
1:C:165:GLY:HA3	1:E:247:GLN:HA	2.00	0.42
1:B:267:ARG:HD2	1:B:271:ASN:ND2	2.34	0.42
1:C:131:ILE:CG2	1:C:132:GLY:N	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ARG:HG2	1:D:166:TRP:HH2	1.84	0.42
1:B:136:VAL:O	1:B:140:MSE:HG2	2.18	0.42
1:D:257:PHE:O	1:D:263:GLY:HA3	2.20	0.42
1:E:277:ASP:C	1:E:277:ASP:OD1	2.58	0.42
1:F:136:VAL:O	1:F:140:MSE:HG2	2.19	0.42
1:F:139:MSE:HE1	1:F:171:MSE:HE3	2.01	0.42
1:F:13:VAL:HG21	1:F:215:VAL:HG21	2.02	0.42
1:A:130:SER:O	1:A:131:ILE:HD12	2.19	0.41
1:B:285:PRO:HG3	1:E:65:TYR:CD1	2.55	0.41
1:E:106:LEU:N	1:E:106:LEU:HD12	2.35	0.41
1:E:60:LEU:HD23	1:E:114:GLN:HG2	2.01	0.41
1:F:105:HIS:CE1	1:F:107:ASN:HB3	2.55	0.41
1:E:20:GLU:HA	1:E:20:GLU:OE2	2.21	0.41
1:C:54[A]:LYS:O	1:C:58:GLN:HG3	2.21	0.41
1:F:57:ILE:HG23	1:F:114:GLN:OE1	2.21	0.41
1:D:60:LEU:HD23	1:D:114:GLN:HG2	2.02	0.41
1:D:277:ASP:O	1:D:280:LYS:HD3	2.21	0.41
1:D:31:THR:HG22	1:D:31:THR:O	2.21	0.41
1:B:70:GLY:CA	1:E:283:ARG:HD3	2.50	0.41
1:E:136:VAL:O	1:E:140:MSE:HG2	2.21	0.41
2:F:286:SO4:O4	4:F:583:HOH:O	2.21	0.41
1:C:106:LEU:C	1:C:106:LEU:HD12	2.40	0.41
1:F:49:ARG:HB2	1:F:50:PRO:HD2	2.03	0.41
1:A:273:LYS:O	4:A:527:HOH:O	2.21	0.40
1:B:159:VAL:CG1	1:B:159:VAL:O	2.70	0.40
1:D:219:ARG:O	1:D:223:GLN:HG2	2.21	0.40
1:E:146:ALA:O	1:E:204:VAL:HA	2.21	0.40
1:C:162:PHE:O	1:E:254[A]:THR:CG2	2.70	0.40
1:C:270:PHE:CD2	1:C:271:ASN:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/288 (93%)	258 (97%)	8 (3%)	1 (0%)	38	32
1	B	262/288 (91%)	255 (97%)	7 (3%)	0	100	100
1	C	263/288 (91%)	254 (97%)	9 (3%)	0	100	100
1	D	264/288 (92%)	258 (98%)	6 (2%)	0	100	100
1	E	264/288 (92%)	252 (96%)	11 (4%)	1 (0%)	38	32
1	F	241/288 (84%)	232 (96%)	8 (3%)	1 (0%)	38	32
All	All	1561/1728 (90%)	1509 (97%)	49 (3%)	3 (0%)	51	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	GLY
1	F	258	TYR
1	E	156	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	220/220 (100%)	218 (99%)	2 (1%)	82	87
1	B	215/220 (98%)	214 (100%)	1 (0%)	91	94
1	C	216/220 (98%)	213 (99%)	3 (1%)	71	77
1	D	217/220 (99%)	215 (99%)	2 (1%)	82	87
1	E	217/220 (99%)	213 (98%)	4 (2%)	64	68
1	F	197/220 (90%)	194 (98%)	3 (2%)	70	75
All	All	1282/1320 (97%)	1267 (99%)	15 (1%)	78	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	280	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	138	HIS
1	C	49	ARG
1	C	138	HIS
1	C	282	LYS
1	D	54	LYS
1	D	138	HIS
1	E	138	HIS
1	E	200	LEU
1	E	267	ARG
1	E	271	ASN
1	F	54[A]	LYS
1	F	54[B]	LYS
1	F	138	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	C	284	ASN
1	E	271	ASN
1	F	193	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	286	-	4,4,4	0.24	0	6,6,6	0.11	0
3	BCT	A	287	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	B	286	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	C	286	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	D	286	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	E	286	-	0,3,3	0.00	-	0,3,3	0.00	-
2	SO4	F	286	-	4,4,4	0.23	0	6,6,6	0.15	0
3	BCT	F	287	-	0,3,3	0.00	-	0,3,3	0.00	-
3	BCT	F	288	-	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	286	-	-	0/0/0/0	0/0/0/0
3	BCT	A	287	-	-	0/0/0/0	0/0/0/0
3	BCT	B	286	-	-	0/0/0/0	0/0/0/0
3	BCT	C	286	-	-	0/0/0/0	0/0/0/0
3	BCT	D	286	-	-	0/0/0/0	0/0/0/0
3	BCT	E	286	-	-	0/0/0/0	0/0/0/0
2	SO4	F	286	-	-	0/0/0/0	0/0/0/0
3	BCT	F	287	-	-	0/0/0/0	0/0/0/0
3	BCT	F	288	-	-	0/0/0/0	0/0/0/0

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	286	SO4	2	0
2	F	286	SO4	2	0
3	F	287	BCT	1	0

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	255/288 (88%)	0.15	13 (5%) 29 36	15, 22, 36, 65	0
1	B	251/288 (87%)	0.31	23 (9%) 10 13	12, 20, 33, 53	0
1	C	251/288 (87%)	0.53	34 (13%) 3 4	15, 21, 41, 65	0
1	D	253/288 (87%)	0.35	19 (7%) 15 19	14, 22, 32, 51	0
1	E	253/288 (87%)	0.21	19 (7%) 15 19	10, 21, 34, 59	0
1	F	228/288 (79%)	0.01	7 (3%) 49 58	6, 17, 29, 44	0
All	All	1491/1728 (86%)	0.26	115 (7%) 14 18	6, 21, 35, 65	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	271	ASN	11.9
1	B	104	HIS	9.2
1	C	270	PHE	8.2
1	A	104	HIS	7.2
1	C	269	ALA	6.7
1	E	105	HIS	6.5
1	C	273	LYS	6.1
1	C	267	ARG	6.0
1	C	272	GLN	5.8
1	C	268	ASN	5.8
1	E	12	PRO	5.6
1	B	282	LYS	5.2
1	D	7	THR	5.0
1	A	273	LYS	5.0
1	A	258	TYR	4.9
1	B	7	THR	4.9
1	C	5	ASP	4.8
1	C	280	LYS	4.8
1	E	271	ASN	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	274	ARG	4.7
1	C	277	ASP	4.6
1	B	270	PHE	4.6
1	C	279	SER	4.4
1	C	281	PHE	4.3
1	C	7	THR	4.1
1	C	282	LYS	4.1
1	D	88	GLN	4.0
1	A	271	ASN	4.0
1	B	258	TYR	4.0
1	C	275	GLN	3.9
1	C	284	ASN	3.9
1	E	270[A]	PHE	3.9
1	F	7	THR	3.8
1	D	5	ASP	3.8
1	B	272	GLN	3.7
1	B	267	ARG	3.6
1	C	258	TYR	3.6
1	E	258	TYR	3.5
1	E	5	ASP	3.5
1	D	6	GLU	3.5
1	D	267	ARG	3.3
1	B	105	HIS	3.3
1	D	87	ASP	3.2
1	C	65	TYR	3.2
1	B	268	ASN	3.2
1	B	11	ALA	3.2
1	B	273	LYS	3.2
1	E	273	LYS	3.2
1	E	275	GLN	3.2
1	A	7	THR	3.1
1	C	264	GLN	3.1
1	D	16	HIS	3.1
1	C	6	GLU	3.1
1	C	266	GLY	3.1
1	C	80	LYS	3.0
1	E	282	LYS	3.0
1	E	143	LEU	3.0
1	C	283	ARG	3.0
1	B	269	ALA	3.0
1	B	271	ASN	3.0
1	F	185	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	275	GLN	3.0
1	D	282	LYS	2.9
1	E	267	ARG	2.9
1	E	10	TYR	2.9
1	C	124	ALA	2.9
1	A	105	HIS	2.9
1	C	285	PRO	2.9
1	C	261	GLU	2.9
1	B	274	ARG	2.9
1	E	6	GLU	2.9
1	D	10	TYR	2.8
1	D	20[A]	GLU	2.8
1	E	272	GLN	2.8
1	C	123	VAL	2.7
1	D	65	TYR	2.7
1	B	281	PHE	2.7
1	A	143	LEU	2.7
1	E	229	LEU	2.7
1	B	280	LYS	2.6
1	F	105	HIS	2.6
1	D	141	CYS	2.6
1	D	14	GLU	2.5
1	F	123	VAL	2.5
1	A	123	VAL	2.4
1	E	87	ASP	2.4
1	B	159	VAL	2.4
1	D	160	GLY	2.4
1	F	87	ASP	2.4
1	C	44	VAL	2.4
1	D	123	VAL	2.4
1	B	113[A]	ARG	2.3
1	E	141	CYS	2.3
1	E	276	PRO	2.3
1	C	45	ARG	2.3
1	C	143	LEU	2.3
1	D	185	PHE	2.3
1	A	124	ALA	2.3
1	B	141	CYS	2.3
1	D	74	LEU	2.3
1	F	5	ASP	2.2
1	B	276	PRO	2.2
1	A	268	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	88	GLN	2.2
1	A	270	PHE	2.2
1	B	158	LYS	2.2
1	B	283	ARG	2.2
1	C	71[A]	VAL	2.1
1	A	5	ASP	2.1
1	C	232	LEU	2.1
1	C	278	PHE	2.1
1	F	6	GLU	2.1
1	D	229	LEU	2.0
1	D	73	ILE	2.0
1	E	73	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	286	5/5	0.91	0.20	5.55	37,39,45,53	5
2	SO4	F	286	5/5	0.91	0.23	5.34	42,42,44,54	5
3	BCT	A	287	4/4	0.91	0.16	2.12	27,30,33,37	0
3	BCT	C	286	4/4	0.94	0.15	0.85	28,33,36,38	0
3	BCT	D	286	4/4	0.95	0.14	0.49	23,29,33,35	0
3	BCT	F	287	4/4	0.96	0.12	0.25	18,27,32,36	0
3	BCT	B	286	4/4	0.94	0.13	-0.77	26,35,38,40	0
3	BCT	E	286	4/4	0.97	0.10	-1.09	22,30,34,36	0
3	BCT	F	288	4/4	0.90	0.22	-	54,54,55,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.