



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:16 AM UTC

PDB ID : 9F00 / pdb_00009f00
Title : Complex between D-SH2 domain of ABL with monobody DAM27
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Deposited on : 2024-04-14
Resolution : 2.91 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

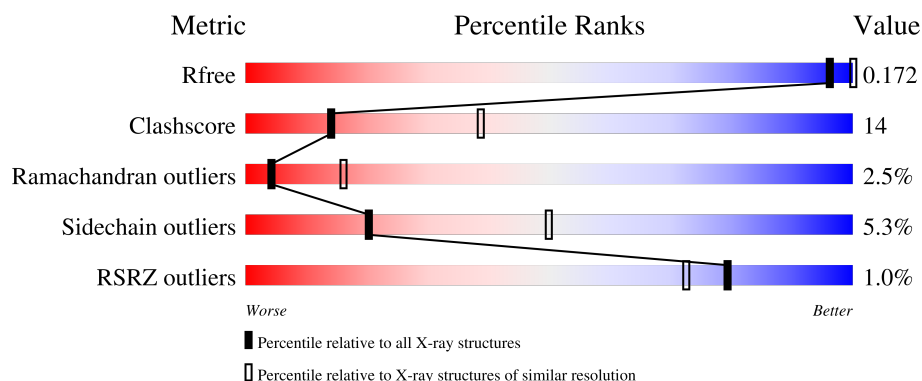
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	99	74% 26%
1	B	99	82% 18%
2	C	98	69% 23% • 5%
2	D	98	2% 67% 28% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3012 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 (with D amino acids) called synthetic D-SH2 domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	0	0
			787	492	145	149	1			
1	B	99	Total	C	N	O	S	0	0	0
			787	492	145	149	1			

- Molecule 2 is a protein called monobody DAM27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	96	Total	C	N	O	S	0	1	0
			724	464	109	150	1			
2	C	93	Total	C	N	O		0	0	0
			701	450	106	145				

- Molecule 3 is water.

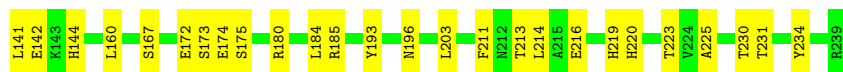
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	5	Total	O	0	0
			5	5		
3	D	3	Total	O	0	0
			3	3		
3	C	2	Total	O	0	0
			2	2		

3 Residue-property plots [i](#)

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

- Molecule 1: synthetic D-SH2 domain

Chain A:  74% 26%



- Molecule 1: synthetic D-SH2 domain

Chain B:  82% 18%



- Molecule 2: monobody DAM27

Chain D:  2% 67% 28%



- Molecule 2: monobody DAM27

Chain C:  69% 23% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	111.33Å 111.33Å 205.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.96 – 2.91 48.96 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.96-2.91) 65.1 (48.96-2.91)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.209 , 0.257 (Not available) , 0.172	Depositor DCC
R_{free} test set	871 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3012	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: DSG, DAS, DTH, DHI, DLE, DLY, DTR, DTY, DCY, DAL, DIL, DPR, DSN, DVA, DGL, DPN, DGN, DAR

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	0.29	0/21	0.62	0/14
1	B	0.24	0/21	0.39	0/14
2	C	0.46	0/721	0.77	0/987
2	D	0.47	0/747	0.82	0/1022
All	All	0.46	0/1510	0.79	0/2037

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	787	0	691	19	0
1	B	787	0	689	12	0
2	C	701	0	666	23	0
2	D	724	0	689	31	0
3	A	3	0	0	0	0
3	B	5	0	0	1	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
All	All	3012	0	2735	82	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 14.

All (82) 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:A:174:DGL:HB2	2:C:83:SER:HB3	1.71	0.72
2:D:14:VAL:HG22	2:D:24:ILE:HG22	1.76	0.68
2:D:39:THR:HB	2:D:75:THR:HG23	1.75	0.68
2:C:39:THR:HB	2:C:75:THR:HG23	1.76	0.67
2:D:18:THR:CG2	2:D:20:THR:HG22	2.31	0.61
1:B:207:DSN:HB2	1:B:210:DAR:HH11	1.66	0.60
1:A:175:DSN:HB3	1:B:194:DAR:NH2	2.17	0.59
2:D:18:THR:HG22	2:D:20:THR:H	1.69	0.58
1:A:219:DHI:O	1:A:223:DTH:HG22	2.03	0.58
1:A:184:DLE:HD13	1:A:193:DTY:HE1	1.86	0.58
2:D:38:ILE:HG13	2:D:76:VAL:HG22	1.85	0.58
2:C:82:TYR:O	2:C:84:GLY:N	2.37	0.57
1:A:180:DAR:NH2	1:A:214:DLE:HD12	2.19	0.56
2:C:70:VAL:O	2:C:98:THR:HG22	2.06	0.56
1:A:141:DLE:O	1:A:142:DGL:HB2	2.06	0.56
2:C:16:ALA:HB3	2:C:23:LEU:HB2	1.88	0.55
1:A:213:DTH:HG23	1:A:216:DGL:CD	2.36	0.55
2:C:8:VAL:HG21	2:C:89:PHE:HD2	1.73	0.54
2:D:18:THR:HG22	2:D:20:THR:HG22	1.88	0.54
2:D:43:THR:HG22	2:D:71:ASP:O	2.08	0.53
2:C:18:THR:HG23	2:C:19:PRO:HD2	1.91	0.53
1:A:230:DTH:HG22	1:A:231:DTH:O	2.09	0.53
2:D:70:VAL:H	2:D:98:THR:CG2	2.21	0.52
2:D:43:THR:HB	2:D:73:THR:HB	1.90	0.52
2:C:70:VAL:H	2:C:98:THR:CG2	2.23	0.52
1:A:211:DPN:HD2	1:A:216:DGL:HB3	1.92	0.52
2:C:52:PHE:C	2:C:52:PHE:CD1	2.89	0.51
2:C:67:LYS:O	2:C:98:THR:HG21	2.10	0.51
2:C:52:PHE:C	2:C:52:PHE:HD1	2.18	0.51
1:B:167:DSN:HA	1:B:234:DTY:O	2.11	0.50
2:D:43:THR:HG22	2:D:71:ASP:C	2.37	0.50
2:C:16:ALA:HB3	2:C:23:LEU:HD22	1.93	0.50
1:A:141:DLE:HD22	1:A:144:DHI:CD2	2.42	0.50
1:B:142:DGL:HG3	1:B:147:DTY:HD2	1.94	0.49
2:C:75:THR:HB	2:C:93:SER:OG	2.13	0.49
2:D:14:VAL:HG23	2:D:94:ILE:HD11	1.94	0.49
2:D:18:THR:HG21	2:D:20:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:38:ILE:HB	2:C:52:PHE:CE1	2.49	0.48
1:B:174:DGL:HG3	2:D:82:TYR:CE1	2.49	0.47
1:B:219:DHI:O	1:B:223:DTH:HG22	2.13	0.47
2:C:43:THR:CG2	2:C:71:ASP:HB3	2.44	0.47
2:D:89:PHE:N	2:D:89:PHE:CD1	2.83	0.47
2:D:19:PRO:O	2:D:98:THR:OG1	2.33	0.47
1:B:176:DSN:HB3	1:B:179:DGN:HG3	1.97	0.47
2:D:69:GLY:N	2:D:98:THR:HG23	2.30	0.47
1:A:225:DAL:N	1:A:231:DTH:HG22	2.30	0.46
1:B:210:DAR:HG2	1:B:210:DAR:HH21	1.80	0.46
2:D:42:GLU:OE2	2:D:67:LYS:HE3	2.15	0.46
2:D:36:TYR:CD1	2:D:36:TYR:N	2.84	0.46
2:C:82:TYR:O	2:C:83:SER:C	2.59	0.45
2:D:67:LYS:O	2:D:98:THR:HG21	2.16	0.45
2:D:82:TYR:O	2:D:84:GLY:N	2.49	0.45
2:C:8:VAL:HG21	2:C:89:PHE:CD2	2.51	0.45
1:A:142:DGL:C	1:A:144:DHI:N	2.79	0.45
1:B:196:DSG:O	1:B:203:DLE:HA	2.17	0.45
2:D:89:PHE:N	2:D:89:PHE:HD1	2.14	0.45
2:C:18:THR:HB	2:C:21:SER:OG	2.17	0.44
2:D:67:LYS:HA	2:D:68:PRO:HD3	1.88	0.44
1:A:167:DSN:HA	1:A:234:DTY:O	2.17	0.44
2:D:22:LEU:HD21	2:D:96:TYR:CE2	2.52	0.44
2:D:70:VAL:H	2:D:98:THR:HG22	1.82	0.44
1:B:197:DTH:HG22	1:B:203:DLE:HB3	1.99	0.44
2:D:77:TYR:HD1	2:D:77:TYR:N	2.16	0.43
1:A:160:DLE:O	1:A:185:DAR:HD2	2.18	0.43
1:A:172:DGL:HB3	1:A:173:DSN:H	1.47	0.43
1:B:213:DTH:O	1:B:216:DGL:HB2	2.20	0.42
1:A:211:DPN:HZ	1:A:220:DHI:CG	2.50	0.42
2:D:96:TYR:CE2	2:D:98:THR:HA	2.55	0.42
2:D:77:TYR:N	2:D:77:TYR:CD1	2.87	0.42
2:C:89:PHE:N	2:C:89:PHE:CD1	2.87	0.42
2:D:82:TYR:O	2:D:83:SER:C	2.63	0.42
2:C:18:THR:HG22	2:C:20:THR:H	1.85	0.42
2:C:42:GLU:HB2	2:C:46:GLY:O	2.20	0.41
2:C:43:THR:HB	2:C:73:THR:HB	2.01	0.41
2:C:89:PHE:N	2:C:89:PHE:HD1	2.18	0.41
1:A:141:DLE:HD22	1:A:144:DHI:HD2	2.03	0.41
1:A:173:DSN:O	1:A:174:DGL:C	2.67	0.41
2:D:36:TYR:N	2:D:36:TYR:HD1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:DSG:O	1:A:203:DLE:HA	2.21	0.41
2:D:7:SER:HA	2:D:90:SER:HB2	2.02	0.40
1:B:239:DAR:HD3	3:B:305:HOH:O	2.21	0.40
2:D:7:SER:HB2	2:D:90:SER:O	2.20	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	7/99 (7%)	7 (100%)	0	0	100	100
1	B	7/99 (7%)	7 (100%)	0	0	100	100
2	C	91/98 (93%)	87 (96%)	2 (2%)	2 (2%)	5	19
2	D	95/98 (97%)	89 (94%)	3 (3%)	3 (3%)	3	12
All	All	200/394 (51%)	190 (95%)	5 (2%)	5 (2%)	4	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	83	SER
2	C	83	SER
2	D	46	GLY
2	C	47	GLY
2	D	18	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	6/79 (8%)	5 (83%)	1 (17%)	2	7
2	D	32/79 (40%)	31 (97%)	1 (3%)	35	67
All	All	38/158 (24%)	36 (95%)	2 (5%)	20	50

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	89	PHE
2	C	52	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

184 non-standard protein/DNA/RNA residues are modelled in this entry.

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.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	7/99 (7%)	-0.18	0	100 100	79, 93, 117, 171	0
1	B	7/99 (7%)	-0.39	0	100 100	60, 70, 110, 148	0
2	C	93/98 (94%)	0.03	0	100 100	62, 75, 100, 135	0
2	D	96/98 (97%)	0.06	2 (2%)	63 54	50, 74, 128, 155	1 (1%)
All	All	203/394 (51%)	0.02	2 (0%)	79 72	50, 75, 127, 171	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	27[A]	ASP	2.5
2	D	24	ILE	2.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	DLY	A	143	5/10	0.54	0.18	140,141,144,147	0
1	DAR	A	239	11/12	0.56	0.20	126,134,145,146	0
1	DSN	A	145	6/7	0.57	0.14	116,125,128,131	0
1	DGL	A	142	9/10	0.63	0.17	138,140,158,159	0
1	DSN	A	176	6/7	0.69	0.15	150,163,165,170	0
1	DTH	A	223	7/8	0.71	0.16	110,112,121,126	0
1	DSN	B	176	6/7	0.71	0.13	142,146,153,159	0
1	DGN	B	179	9/10	0.72	0.14	103,124,138,140	0
1	DTH	A	231	7/8	0.75	0.13	101,102,108,110	0
1	DHI	B	144	10/11	0.76	0.15	102,105,110,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	DLY	A	238	9/10	0.76	0.14	108,114,131,132	0
1	DGN	A	179	9/10	0.76	0.17	114,133,138,143	0
1	DTH	B	223	7/8	0.78	0.13	93,94,99,101	0
1	DAR	B	239	11/12	0.78	0.18	77,80,87,91	0
1	DSN	B	162	6/7	0.79	0.09	61,68,69,80	0
1	DSN	B	175	6/7	0.81	0.12	137,158,160,163	0
1	DPR	A	177	7/8	0.81	0.11	140,149,156,160	0
1	DGL	A	208	9/10	0.81	0.15	148,157,173,179	0
1	DCY	A	198	6/7	0.82	0.14	112,114,116,120	0
1	DLE	A	141	8/9	0.82	0.22	120,132,139,143	0
1	DSG	A	212	8/9	0.83	0.10	128,133,136,137	0
1	DSN	A	207	6/7	0.83	0.15	132,137,143,143	0
1	DGL	B	174	9/10	0.83	0.12	86,92,121,124	0
1	DTH	A	230	7/8	0.83	0.13	88,92,98,98	0
1	DSN	B	207	6/7	0.84	0.09	112,116,123,130	0
1	DGL	B	142	9/10	0.84	0.17	107,116,125,138	0
1	DGL	B	208	9/10	0.85	0.10	123,131,147,159	0
1	DSN	A	162	6/7	0.85	0.11	101,108,112,115	0
1	DHI	A	233	10/11	0.85	0.12	103,117,123,124	0
1	DSN	A	206	6/7	0.86	0.14	110,115,123,125	0
1	DSN	B	206	6/7	0.86	0.12	99,114,117,125	0
1	DHI	A	144	10/11	0.86	0.12	132,135,141,142	0
1	DSN	A	199	6/7	0.86	0.12	117,123,125,126	0
1	DSN	B	199	6/7	0.86	0.12	107,109,111,112	0
1	DSN	B	209	6/7	0.87	0.11	108,110,117,123	0
1	DGL	B	172	9/10	0.87	0.10	86,90,104,108	0
1	DHI	A	219	10/11	0.87	0.11	120,129,143,144	0
1	DSN	A	173	6/7	0.87	0.10	98,114,115,124	0
1	DGL	A	172	9/10	0.87	0.12	87,97,114,118	0
1	DAS	B	226	8/9	0.87	0.14	84,87,95,97	0
1	DTH	A	197	7/8	0.88	0.14	102,107,110,111	0
1	DPR	B	177	7/8	0.88	0.12	122,133,146,147	0
1	DAR	A	210	11/12	0.88	0.18	116,120,133,135	0
1	DLY	B	143	5/10	0.88	0.12	110,110,112,115	0
1	DTH	B	213	7/8	0.88	0.07	98,100,105,106	0
1	DSN	B	145	6/7	0.88	0.11	84,89,91,99	0
1	DSN	B	222	6/7	0.88	0.07	89,93,94,102	0
1	DAS	B	200	8/9	0.88	0.10	107,111,113,114	0
1	DSG	A	196	8/9	0.89	0.10	96,101,106,106	0
1	DSG	A	165	8/9	0.89	0.11	93,96,99,102	0
1	DSN	A	175	6/7	0.89	0.14	125,130,148,150	0
1	DSG	B	212	8/9	0.89	0.08	106,109,112,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	DAS	A	226	8/9	0.89	0.09	100,103,109,109	0
1	DGL	A	174	9/10	0.89	0.09	97,98,125,139	0
1	DHI	B	219	10/11	0.90	0.10	98,108,130,135	0
1	DAL	A	215	5/6	0.90	0.15	113,114,116,118	0
1	DLY	B	202	9/10	0.90	0.13	105,110,121,126	0
1	DTH	B	230	7/8	0.91	0.13	68,72,77,77	0
1	DAR	A	180	11/12	0.91	0.12	93,108,116,117	0
1	DGL	B	216	9/10	0.91	0.08	94,100,108,109	0
1	DLE	B	141	8/9	0.91	0.19	97,113,121,123	0
1	DTH	A	213	7/8	0.91	0.10	117,122,123,124	0
1	DAR	B	210	11/12	0.91	0.11	105,113,116,119	0
1	DTY	B	204	12/13	0.92	0.10	88,95,102,105	0
1	DSN	B	181	6/7	0.92	0.10	70,72,76,78	0
1	DTH	B	231	7/8	0.92	0.11	77,83,87,90	0
1	DGL	A	187	9/10	0.92	0.09	80,83,89,92	0
1	DAR	A	171	11/12	0.92	0.10	74,82,88,93	0
1	DSG	B	196	8/9	0.92	0.09	83,89,91,92	0
1	DAR	B	180	11/12	0.92	0.12	83,96,107,108	0
1	DHI	A	220	10/11	0.93	0.10	109,114,121,122	0
1	DSN	A	161	6/7	0.93	0.08	92,94,100,103	0
1	DTY	B	147	12/13	0.93	0.13	81,89,96,98	0
1	DGL	A	216	9/10	0.93	0.10	119,123,132,133	0
1	DHI	B	233	10/11	0.93	0.08	73,78,81,82	0
1	DTY	B	234	12/13	0.93	0.08	72,75,78,81	0
1	DPR	A	237	7/8	0.93	0.11	112,113,116,117	0
1	DVA	B	205	7/8	0.93	0.17	83,88,95,96	0
1	DSN	B	173	6/7	0.93	0.13	96,106,116,121	0
1	DLY	A	202	9/10	0.93	0.11	110,114,126,127	0
1	DTY	A	186	12/13	0.94	0.11	80,83,86,89	0
1	DSN	A	209	6/7	0.94	0.09	123,124,129,135	0
1	DVA	A	205	7/8	0.94	0.15	89,102,104,108	0
1	DSN	B	161	6/7	0.94	0.08	57,61,69,72	0
1	DAR	A	194	11/12	0.94	0.09	83,87,99,100	0
1	DPN	A	211	11/12	0.94	0.10	117,120,123,124	0
1	DSN	A	222	6/7	0.94	0.08	109,110,113,121	0
1	DTY	A	234	12/13	0.94	0.09	107,118,126,127	0
1	DAS	A	200	8/9	0.94	0.10	123,127,130,131	0
1	DSN	A	181	6/7	0.94	0.09	81,84,86,93	0
1	DTY	A	147	12/13	0.94	0.09	103,108,110,111	0
1	DLY	B	238	9/10	0.94	0.13	75,76,83,89	0
1	DAL	A	225	5/6	0.94	0.09	94,99,101,107	0
1	DAR	A	185	11/12	0.94	0.12	82,85,100,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	DTY	A	204	12/13	0.95	0.12	103,109,115,115	0
1	DSN	A	183	6/7	0.95	0.10	72,77,80,83	0
1	DTH	B	197	7/8	0.95	0.11	92,98,103,104	0
1	DHI	A	221	10/11	0.95	0.09	99,104,109,113	0
1	DTR	B	146	14/15	0.95	0.12	77,87,92,95	0
1	DCY	B	198	6/7	0.95	0.08	103,104,110,117	0
1	DPR	A	150	7/8	0.95	0.07	86,92,93,96	0
1	DAR	A	153	11/12	0.95	0.12	70,75,84,84	0
1	DAR	B	153	11/12	0.95	0.12	62,67,73,74	0
1	DAR	B	194	11/12	0.95	0.07	72,78,84,87	0
1	DSG	A	154	8/9	0.95	0.10	71,73,74,76	0
1	DGL	B	157	9/10	0.95	0.10	57,61,67,68	0
1	DIL	B	229	8/9	0.96	0.14	63,66,71,75	0
1	DPN	B	211	11/12	0.96	0.07	99,104,109,109	0
1	DLE	B	203	8/9	0.96	0.11	89,97,99,103	0
1	DIL	A	164	8/9	0.96	0.09	99,103,107,111	0
1	DVA	A	151	7/8	0.96	0.09	80,83,85,87	0
1	DSN	B	152	6/7	0.96	0.07	67,68,69,69	0
1	DAR	B	185	11/12	0.96	0.07	58,62,68,69	0
1	DAL	B	215	5/6	0.96	0.11	92,94,98,99	0
1	DVA	B	224	7/8	0.96	0.08	89,91,93,96	0
1	DPR	B	235	7/8	0.96	0.09	71,74,76,79	0
1	DSG	B	154	8/9	0.96	0.07	61,65,66,69	0
1	DPR	B	237	7/8	0.96	0.09	70,71,75,75	0
1	DAL	B	225	5/6	0.96	0.07	79,81,83,91	0
1	DHI	B	148	10/11	0.96	0.06	69,75,81,82	0
1	DGL	B	187	9/10	0.96	0.07	61,61,72,75	0
1	DIL	A	229	8/9	0.96	0.12	81,86,91,98	0
1	DTY	A	191	12/13	0.97	0.06	70,72,77,77	0
1	DLE	A	203	8/9	0.97	0.10	104,107,110,111	0
1	DTY	B	191	12/13	0.97	0.12	59,62,64,67	0
1	DTY	B	193	12/13	0.97	0.08	65,66,71,71	0
1	DSG	B	165	8/9	0.97	0.06	65,66,71,71	0
1	DTR	A	146	14/15	0.97	0.10	105,110,115,117	0
1	DIL	A	195	8/9	0.97	0.10	84,88,96,99	0
1	DAR	B	171	11/12	0.97	0.11	68,71,83,84	0
1	DSN	A	152	6/7	0.97	0.04	74,76,81,84	0
1	DLE	A	184	8/9	0.97	0.10	75,80,83,86	0
1	DHI	A	148	10/11	0.97	0.07	90,95,100,104	0
1	DPR	B	150	7/8	0.97	0.08	75,80,82,83	0
1	DHI	B	220	10/11	0.97	0.07	95,101,104,105	0
1	DTY	A	158	12/13	0.97	0.10	81,85,92,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	DPR	A	235	7/8	0.97	0.08	111,114,117,117	0
1	DHI	B	221	10/11	0.97	0.08	83,91,95,96	0
1	DIL	B	164	8/9	0.97	0.08	65,69,72,74	0
1	DLE	A	159	8/9	0.97	0.12	82,88,96,98	0
1	DAR	A	189	11/12	0.97	0.07	69,72,75,79	0
1	DAR	B	189	11/12	0.97	0.08	57,61,63,64	0
1	DVA	A	224	7/8	0.97	0.09	106,108,113,114	0
1	DVA	B	190	7/8	0.97	0.12	57,60,62,64	0
1	DHI	B	192	10/11	0.98	0.07	64,66,67,67	0
1	DTY	A	193	12/13	0.98	0.09	75,77,83,83	0
1	DPN	A	168	11/12	0.98	0.07	90,94,100,101	0
1	DLE	A	214	8/9	0.98	0.11	99,106,112,117	0
1	DSN	B	183	6/7	0.98	0.05	61,62,67,68	0
1	DPN	B	168	11/12	0.98	0.09	66,68,76,76	0
1	DLE	A	169	8/9	0.98	0.09	79,84,89,89	0
1	DIL	B	195	8/9	0.98	0.09	74,77,83,85	0
1	DLE	A	217	8/9	0.98	0.10	94,111,118,118	0
1	DLE	B	217	8/9	0.98	0.09	87,94,95,96	0
1	DLE	B	169	8/9	0.98	0.09	63,66,72,72	0
1	DAL	B	155	5/6	0.98	0.07	61,62,63,70	0
1	DTY	B	186	12/13	0.98	0.12	59,64,67,75	0
1	DTY	B	158	12/13	0.98	0.09	58,63,70,82	0
1	DAL	A	156	5/6	0.98	0.09	73,74,77,77	0
1	DLE	A	160	8/9	0.98	0.15	81,86,94,101	0
1	DGL	A	157	9/10	0.98	0.08	69,72,81,83	0
1	DVA	A	190	7/8	0.98	0.11	71,71,73,77	0
1	DAL	A	155	5/6	0.98	0.05	76,76,78,80	0
1	DSN	A	167	6/7	0.98	0.06	92,96,99,101	0
1	DSN	B	167	6/7	0.98	0.06	65,67,69,70	0
1	DHI	A	192	10/11	0.98	0.08	72,73,75,77	0
1	DVA	B	151	7/8	0.99	0.07	69,70,72,74	0
1	DLE	B	159	8/9	0.99	0.06	59,61,64,64	0
1	DLE	A	232	8/9	0.99	0.13	97,99,107,108	0
1	DLE	B	232	8/9	0.99	0.11	74,78,83,89	0
1	DVA	A	218	7/8	0.99	0.07	103,108,115,117	0
1	DVA	B	218	7/8	0.99	0.09	87,89,95,99	0
1	DVA	A	170	7/8	0.99	0.08	84,87,91,92	0
1	DLE	B	184	8/9	0.99	0.07	61,62,66,70	0
1	DVA	B	170	7/8	0.99	0.08	72,73,77,78	0
1	DLE	B	214	8/9	0.99	0.08	84,89,95,99	0
1	DAL	A	236	5/6	0.99	0.07	101,108,112,114	0
1	DAL	B	236	5/6	0.99	0.07	70,71,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	DLE	A	228	8/9	0.99	0.08	80,89,92,93	0
1	DLE	B	228	8/9	0.99	0.08	70,72,73,78	0
1	DAL	B	156	5/6	0.99	0.05	60,61,63,64	0
1	DLE	B	160	8/9	0.99	0.07	58,60,62,63	0
1	DIL	A	182	8/9	0.99	0.09	77,80,82,85	0
1	DIL	B	182	8/9	0.99	0.09	65,65,73,73	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.