



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:09 PM UTC

PDB ID : 6NDX / pdb_00006ndx
Title : Lysinoalanine cross-linked FlgE dimer from *Treponema denticola*
Authors : Lynch, M.J.; Crane, B.R.
Deposited on : 2018-12-14
Resolution : 3.04 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

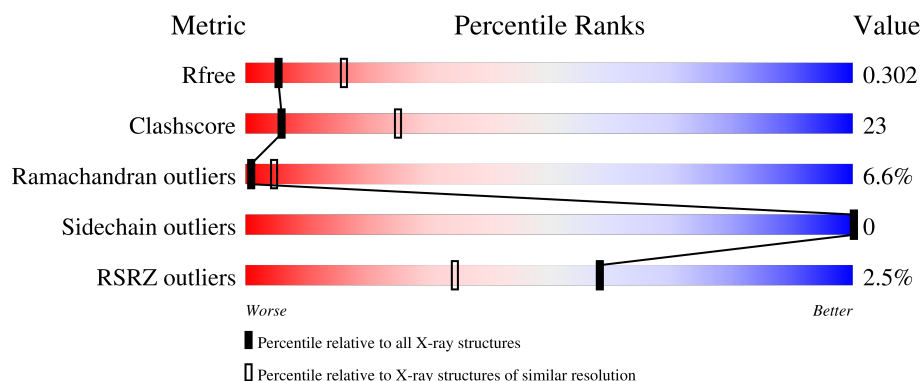
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	3685 (3.08-3.00)
Clashscore	190562	4007 (3.08-3.00)
Ramachandran outliers	187476	3834 (3.08-3.00)
Sidechain outliers	187428	3836 (3.08-3.00)
RSRZ outliers	180081	3684 (3.08-3.00)

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	333	4% 30% 25% 5% 40%
1	B	333	42% 22% • 35%
2	C	177	2% 61% 31% 5% • •
2	D	177	• 62% 31% 5% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5774 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 Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	B	218	Total	C	N	O	0	0	0
			1657	1027	288	342			
1	A	201	Total	C	N	O	0	0	0
			1528	948	267	313			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	ALA	CYS	engineered mutation	UNP Q9RQB6
A	11	ALA	CYS	engineered mutation	UNP Q9RQB6

- Molecule 2 is a protein called Flagellar hook protein FlgE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	171	Total	C	N	O	0	0	0
			1290	796	227	267			
2	D	172	Total	C	N	O	0	0	0
			1294	798	227	269			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	DAL	CYS	conflict	UNP Q9RQB6
D	11	DAL	CYS	conflict	UNP Q9RQB6

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	O	0	0
			2	2		
3	A	1	Total	O	0	0
			1	1		

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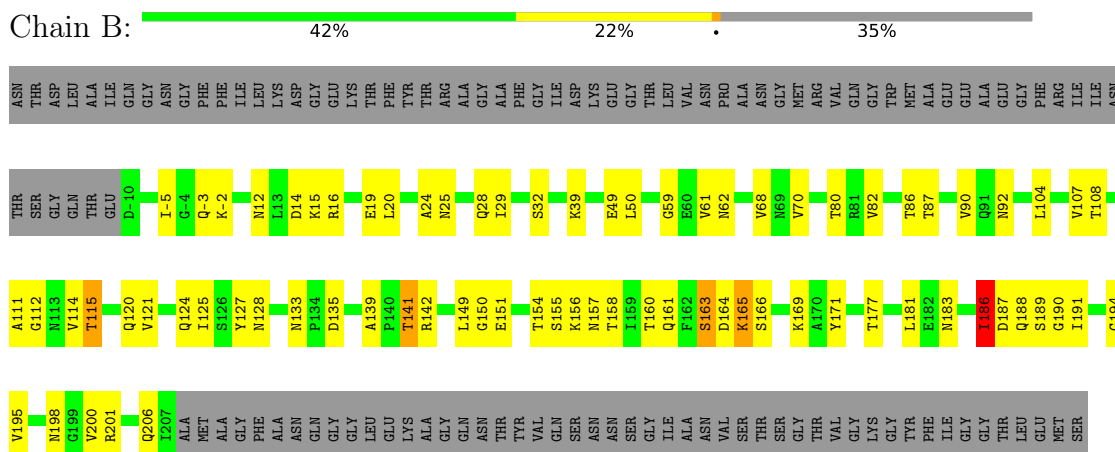
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	O	0	0
			2	2		

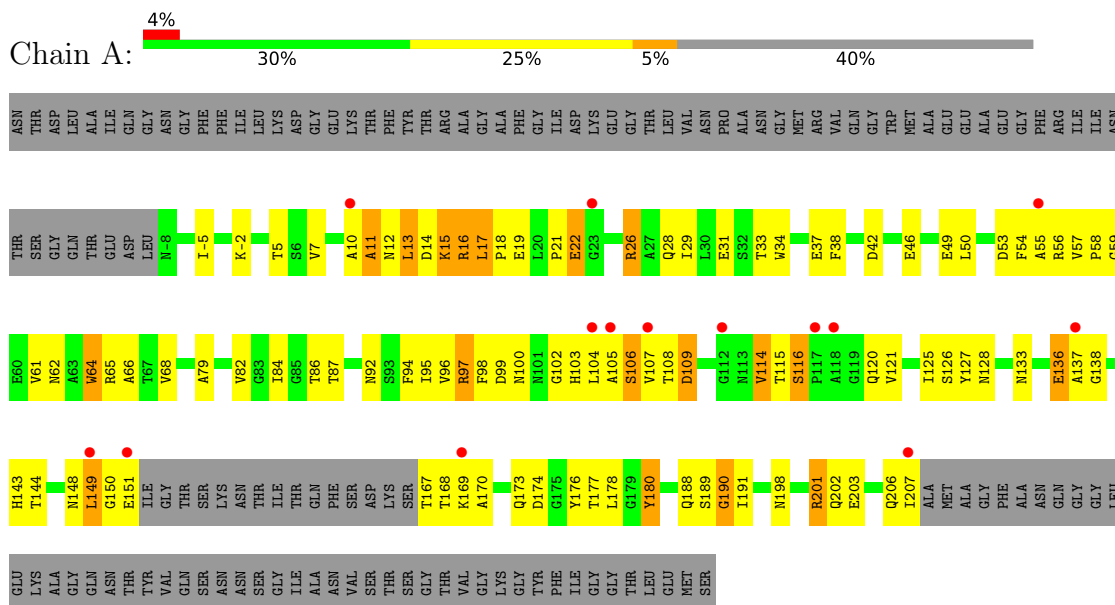
3 Residue-property plots

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: Flagellar hook protein FlgE

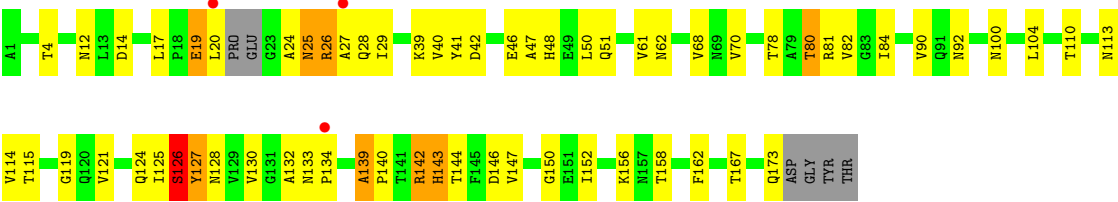


• Molecule 1: Flagellar hook protein FlgE

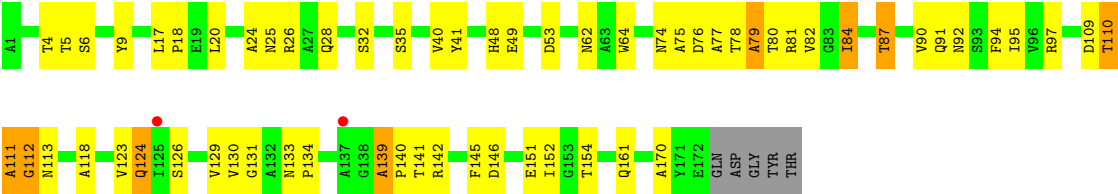


• Molecule 2: Flagellar hook protein FlgE





● Molecule 2: Flagellar hook protein FlgE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	41.56Å 136.35Å 112.18Å 90.00° 96.53° 90.00°	Depositor
Resolution (Å)	43.10 – 3.04 43.10 – 3.04	Depositor EDS
% Data completeness (in resolution range)	89.7 (43.10-3.04) 93.7 (43.10-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.248 , 0.316 0.238 , 0.302	Depositor DCC
R_{free} test set	1986 reflections (6.71%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 30.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5774	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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

5.1 Standard geometry

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

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	0.73	5/1555 (0.3%)	1.13	15/2121 (0.7%)
1	B	0.50	0/1686	0.84	2/2299 (0.1%)
2	C	0.48	0/1306	0.85	1/1780 (0.1%)
2	D	0.60	2/1312 (0.2%)	0.99	10/1791 (0.6%)
All	All	0.59	7/5859 (0.1%)	0.96	28/7991 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	ARG	CB-CG	11.59	1.87	1.52
1	A	26	ARG	NE-CZ	9.58	1.43	1.33
1	A	26	ARG	CG-CD	8.53	1.78	1.52
1	A	26	ARG	CA-CB	6.28	1.64	1.53
2	D	113	ASN	CA-CB	5.68	1.60	1.53
1	A	114	VAL	CB-CG2	-5.51	1.34	1.52
2	D	112	GLY	CA-C	5.08	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	ILE	CA-C-N	11.24	139.80	122.94
1	B	186	ILE	C-N-CA	11.24	139.80	122.94
1	A	26	ARG	NE-CZ-NH1	11.04	132.54	121.50
1	A	97	ARG	CA-CB-CG	10.19	134.48	114.10
1	A	26	ARG	CD-NE-CZ	9.70	137.98	124.40
1	A	26	ARG	CA-CB-CG	9.38	132.87	114.10
1	A	26	ARG	NH1-CZ-NH2	-9.00	107.60	119.30
1	A	26	ARG	CB-CG-CD	8.56	130.98	111.30
1	A	97	ARG	CB-CA-C	-8.40	99.13	111.91
2	D	113	ASN	CA-CB-CG	8.36	120.96	112.60
1	A	97	ARG	CB-CG-CD	8.19	130.14	111.30
1	A	97	ARG	NE-CZ-NH2	7.26	125.73	119.20
2	D	113	ASN	N-CA-CB	6.24	120.04	109.87
1	A	26	ARG	CG-CD-NE	6.24	125.72	112.00
1	A	109	ASP	N-CA-C	6.19	116.62	108.07
2	C	126	SER	N-CA-C	6.17	123.94	110.80
2	D	113	ASN	CA-C-N	-5.98	113.84	122.45
2	D	113	ASN	C-N-CA	-5.98	113.84	122.45
1	A	96	VAL	CA-C-N	5.95	131.01	122.21
1	A	96	VAL	C-N-CA	5.95	131.01	122.21
2	D	111	ALA	CA-C-N	5.78	132.74	121.41
2	D	111	ALA	C-N-CA	5.78	132.74	121.41
1	A	109	ASP	CB-CA-C	-5.77	101.14	114.41
2	D	49	GLU	CG-CD-OE1	5.72	131.57	118.40
2	D	87	THR	CA-C-N	-5.65	112.14	121.92
2	D	87	THR	C-N-CA	-5.65	112.14	121.92
2	D	49	GLU	CG-CD-OE2	-5.19	106.45	118.40
1	A	22	GLU	CA-CB-CG	5.15	124.39	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	99	ASP	Peptide
1	B	186	ILE	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1528	0	1459	109	1
1	B	1657	0	1589	56	0
2	C	1290	0	1232	60	0
2	D	1294	0	1229	41	1
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
All	All	5774	0	5509	258	1

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 23.

All (258) 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:26:ARG:CD	1:A:26:ARG:CG	1.78	1.58
1:A:26:ARG:CG	1:A:26:ARG:CB	1.87	1.50
1:A:14:ASP:CG	1:A:15:LYS:HE3	1.64	1.22
1:A:107:VAL:HG12	1:A:114:VAL:HG12	1.12	1.07
1:A:107:VAL:HG12	1:A:114:VAL:CG1	1.89	1.02
1:B:160:THR:HG23	1:B:169:LYS:NZ	1.74	1.00
2:C:39:LYS:O	2:C:173:GLN:NE2	2.01	0.92
2:C:150:GLY:HA3	2:C:158:THR:HG23	1.53	0.91
2:C:104:LEU:HD21	2:C:121:VAL:HG21	1.53	0.89
1:A:107:VAL:CG1	1:A:114:VAL:HG12	1.99	0.88
1:A:62:ASN:ND2	1:A:98:PHE:O	2.06	0.87
2:C:12:ASN:H	2:C:167:THR:HG23	1.37	0.86
2:C:14:ASP:HB3	2:C:17:LEU:HD13	1.59	0.84
1:B:120:GLN:HG2	1:B:151:GLU:HB3	1.58	0.84
2:C:78:THR:OG1	2:C:128:ASN:N	2.10	0.83
2:D:91:GLN:HG3	2:D:110:THR:HG21	1.60	0.82
2:C:82:VAL:HG12	2:C:125:ILE:HD13	1.62	0.82
2:C:126:SER:O	2:C:144:THR:OG1	1.96	0.81
1:B:160:THR:HG23	1:B:169:LYS:HZ2	1.46	0.80
1:A:57:VAL:O	1:A:59:GLY:N	2.14	0.80
1:A:14:ASP:OD1	1:A:15:LYS:HE3	1.82	0.78
1:A:97:ARG:HB2	1:A:106:SER:HB2	1.66	0.77
1:A:14:ASP:CG	1:A:15:LYS:CE	2.55	0.74
2:C:125:ILE:O	2:C:144:THR:HG23	1.87	0.74
1:A:177:THR:HG22	1:A:178:LEU:H	1.52	0.74
1:B:128:ASN:OD1	1:B:142:ARG:NH2	2.21	0.73
1:A:104:LEU:HG	1:A:105:ALA:H	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:VAL:HG11	2:C:127:TYR:HB3	1.71	0.72
1:B:187:ASP:OD1	1:B:191:ILE:HB	1.89	0.72
1:A:95:ILE:HG13	1:A:108:THR:HG22	1.70	0.72
1:B:108:THR:HG23	1:B:114:VAL:HG22	1.72	0.71
1:A:5:THR:OG1	1:A:174:ASP:OD2	2.09	0.71
1:A:168:THR:HG22	1:A:170:ALA:H	1.55	0.71
1:A:97:ARG:HG2	1:A:97:ARG:HH11	1.54	0.70
2:C:80:THR:HA	2:C:126:SER:OG	1.91	0.70
2:C:81:ARG:H	2:C:126:SER:HB3	1.54	0.70
1:A:-5:ILE:HD12	2:C:156:LYS:NZ	2.06	0.70
1:B:120:GLN:HA	1:B:151:GLU:HA	1.73	0.70
1:A:95:ILE:HG13	1:A:108:THR:CG2	2.21	0.70
1:A:178:LEU:HD13	2:C:162:PHE:CD2	2.26	0.69
1:A:11:ALA:HB2	1:A:168:THR:OG1	1.92	0.69
1:A:97:ARG:CB	1:A:106:SER:HB2	2.23	0.68
2:D:130:VAL:HG12	2:D:131:GLY:H	1.58	0.68
2:D:35:SER:OG	2:D:53:ASP:OD2	2.11	0.68
2:C:126:SER:OG	2:C:127:TYR:N	2.17	0.68
1:A:-5:ILE:HD12	2:C:156:LYS:HZ3	1.59	0.68
1:A:16:ARG:HH11	1:A:103:HIS:H	1.42	0.68
1:B:104:LEU:HD21	1:B:121:VAL:HG11	1.75	0.67
1:B:133:ASN:OD1	2:D:62:ASN:ND2	2.27	0.67
1:A:15:LYS:O	1:A:16:ARG:HG2	1.96	0.66
2:D:75:ALA:O	2:D:77:ALA:N	2.29	0.66
2:C:26:ARG:HG3	2:C:28:GLN:HB2	1.78	0.66
1:A:-2:LYS:HG2	1:A:178:LEU:HD11	1.79	0.65
1:A:189:SER:O	1:A:191:ILE:N	2.30	0.65
1:A:190:GLY:HA3	1:A:207:ILE:HB	1.79	0.65
2:D:64:TRP:HE1	2:D:161:GLN:HE21	1.44	0.65
1:B:14:ASP:HB2	1:B:166:SER:HB2	1.79	0.65
1:B:12:ASN:ND2	1:B:165:LYS:O	2.29	0.64
2:C:81:ARG:H	2:C:126:SER:CB	2.11	0.63
1:B:39:LYS:O	1:B:171:TYR:OH	2.15	0.63
1:A:10:ALA:HB3	1:A:168:THR:CG2	2.29	0.63
1:A:16:ARG:HG2	1:A:103:HIS:CE1	2.34	0.62
1:A:55:ALA:O	1:A:65:ARG:N	2.20	0.62
2:D:40:VAL:HG11	2:D:145:PHE:HZ	1.63	0.62
1:B:160:THR:HG23	1:B:169:LYS:HZ1	1.65	0.62
2:D:4:THR:O	2:D:6:SER:N	2.31	0.62
2:C:127:TYR:HH	2:C:143:HIS:CD2	2.18	0.61
1:A:106:SER:OG	1:A:106:SER:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ALA:HB3	1:A:168:THR:HG21	1.82	0.61
1:A:115:THR:O	1:A:116:SER:OG	2.14	0.61
2:D:64:TRP:HE1	2:D:161:GLN:NE2	1.99	0.61
1:A:14:ASP:O	1:A:15:LYS:HD2	2.00	0.60
1:B:-5:ILE:HA	1:B:181:LEU:HD12	1.83	0.60
1:B:163:SER:OG	1:B:164:ASP:N	2.33	0.60
1:A:95:ILE:O	1:A:108:THR:HB	2.02	0.60
1:B:154:THR:OG1	1:B:155:SER:N	2.34	0.60
1:A:29:ILE:O	1:A:33:THR:HG22	2.01	0.60
2:D:87:THR:HG21	2:D:126:SER:OG	2.02	0.60
1:A:82:VAL:HG11	1:A:94:PHE:HD2	1.67	0.59
1:A:121:VAL:HG22	1:A:149:LEU:HD23	1.84	0.59
2:C:128:ASN:HD22	2:C:140:PRO:HB2	1.67	0.59
2:D:9:TYR:CZ	2:D:170:ALA:HB2	2.37	0.59
1:A:104:LEU:HG	1:A:105:ALA:N	2.17	0.58
1:A:38:PHE:CZ	1:A:50:LEU:HD22	2.39	0.58
2:D:24:ALA:HB1	2:D:28:GLN:HB2	1.85	0.57
2:C:4:THR:HG21	2:C:40:VAL:HG23	1.85	0.57
2:D:87:THR:O	2:D:87:THR:HG22	2.04	0.57
1:B:155:SER:O	1:B:157:ASN:N	2.37	0.57
1:B:82:VAL:HG12	1:B:92:ASN:HA	1.85	0.57
1:A:16:ARG:HG2	1:A:103:HIS:HE1	1.68	0.57
1:A:178:LEU:HD13	2:C:162:PHE:CE2	2.39	0.57
2:D:139:ALA:HB1	2:D:140:PRO:HD2	1.85	0.57
1:A:12:ASN:ND2	1:A:151:GLU:OE2	2.38	0.56
2:C:78:THR:C	2:C:80:THR:H	2.13	0.56
2:D:151:GLU:HG3	2:D:154:THR:CG2	2.35	0.56
2:C:27:ALA:HA	2:C:29:ILE:HD12	1.88	0.56
1:A:19:GLU:O	1:A:56:ARG:NH1	2.39	0.56
2:C:119:GLY:O	2:C:152:ILE:HG13	2.06	0.56
1:A:97:ARG:HB2	1:A:106:SER:CB	2.34	0.55
1:A:10:ALA:HB1	1:A:151:GLU:H	1.71	0.55
2:C:133:ASN:ND2	2:C:139:ALA:O	2.39	0.55
1:B:50:LEU:C	1:B:50:LEU:HD23	2.32	0.55
1:A:177:THR:HG22	1:A:178:LEU:N	2.22	0.54
2:D:95:ILE:HG22	2:D:97:ARG:HE	1.71	0.54
1:B:190:GLY:O	1:B:206:GLN:HA	2.07	0.54
2:C:80:THR:O	2:C:92:ASN:HB3	2.07	0.54
1:B:19:GLU:HG3	1:B:61:VAL:HG22	1.90	0.54
2:C:78:THR:HG1	2:C:128:ASN:H	1.51	0.54
2:C:82:VAL:CG1	2:C:125:ILE:HD13	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:127:TYR:OH	2:C:143:HIS:NE2	2.31	0.53
1:B:80:THR:O	1:B:92:ASN:HB3	2.08	0.53
2:D:20:LEU:HD11	2:D:32:SER:HB2	1.90	0.53
2:C:61:VAL:HG23	2:C:62:ASN:ND2	2.24	0.53
1:B:15:LYS:HG3	1:B:161:GLN:HE21	1.74	0.53
2:D:152:ILE:HD12	2:D:152:ILE:O	2.09	0.53
1:B:90:VAL:HG12	1:B:111:ALA:HB2	1.91	0.53
1:A:103:HIS:HA	1:A:151:GLU:OE1	2.09	0.53
1:A:168:THR:HG22	1:A:169:LYS:N	2.22	0.53
1:A:22:GLU:OE2	1:A:59:GLY:HA3	2.09	0.52
1:A:201:ARG:HB2	1:A:201:ARG:HH11	1.73	0.52
1:A:206:GLN:HG3	1:A:207:ILE:N	2.23	0.52
1:A:13:LEU:HD11	1:A:34:TRP:CD1	2.45	0.52
1:B:177:THR:O	1:B:198:ASN:ND2	2.42	0.52
1:A:-5:ILE:HA	2:C:156:LYS:NZ	2.25	0.52
1:A:97:ARG:HG2	1:A:97:ARG:NH1	2.21	0.52
1:A:107:VAL:HG11	1:A:115:THR:O	2.11	0.51
1:A:125:ILE:O	1:A:144:THR:HA	2.10	0.51
2:D:84:ILE:N	2:D:123:VAL:O	2.41	0.51
2:C:12:ASN:H	2:C:167:THR:CG2	2.15	0.51
2:D:95:ILE:CG2	2:D:97:ARG:HE	2.23	0.51
2:D:90:VAL:HG13	2:D:110:THR:HB	1.91	0.51
2:D:74:ASN:OD1	2:D:77:ALA:HB3	2.11	0.51
1:B:68:VAL:HG11	1:B:125:ILE:HD13	1.91	0.51
2:C:70:VAL:CG1	2:C:127:TYR:HB3	2.39	0.51
1:B:195:VAL:HG12	1:B:201:ARG:HG3	1.93	0.51
2:C:78:THR:CB	2:C:127:TYR:HA	2.40	0.50
1:A:33:THR:HB	1:A:55:ALA:HA	1.93	0.50
1:A:68:VAL:HG11	1:A:82:VAL:CG2	2.42	0.50
1:A:42:ASP:OD2	1:A:46:GLU:HB3	2.11	0.50
1:B:149:LEU:O	1:B:158:THR:HA	2.11	0.50
1:B:150:GLY:HA3	1:B:158:THR:HG23	1.94	0.50
2:C:68:VAL:HG11	2:C:125:ILE:HD12	1.94	0.50
2:C:125:ILE:HG13	2:C:147:VAL:HG13	1.93	0.50
1:B:183:ASN:O	1:B:195:VAL:HG22	2.11	0.50
1:A:190:GLY:O	1:A:207:ILE:N	2.44	0.50
1:A:28:GLN:HA	1:A:31:GLU:HG2	1.94	0.49
1:A:107:VAL:HG11	1:A:115:THR:C	2.36	0.49
1:A:37:GLU:HG2	1:A:49:GLU:HG2	1.94	0.49
2:C:78:THR:OG1	2:C:127:TYR:HA	2.13	0.49
2:C:42:ASP:OD2	2:C:48:HIS:NE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ALA:HB3	1:A:128:ASN:OD1	2.13	0.49
2:D:151:GLU:HG3	2:D:154:THR:HG21	1.93	0.49
1:A:133:ASN:HB2	2:C:100:ASN:HD21	1.78	0.48
1:A:97:ARG:O	1:A:106:SER:HB2	2.13	0.48
2:C:4:THR:HG21	2:C:40:VAL:CG2	2.42	0.48
2:C:125:ILE:C	2:C:144:THR:HG23	2.38	0.48
2:D:77:ALA:C	2:D:79:ALA:H	2.21	0.48
1:A:168:THR:HG22	1:A:170:ALA:N	2.27	0.48
1:A:127:TYR:CE2	1:A:143:HIS:HB3	2.49	0.48
1:B:20:LEU:CD1	1:B:32:SER:HB2	2.43	0.48
1:A:13:LEU:HB2	1:A:17:LEU:HD11	1.94	0.48
1:B:160:THR:CG2	1:B:169:LYS:HZ2	2.22	0.48
1:A:180:TYR:OH	2:C:167:THR:HG21	2.13	0.48
2:D:118:ALA:HA	2:D:152:ILE:HG12	1.95	0.48
1:B:70:VAL:HG21	1:B:127:TYR:CD2	2.49	0.47
1:A:56:ARG:HH21	1:A:62:ASN:HA	1.78	0.47
1:A:120:GLN:HA	1:A:149:LEU:HD21	1.96	0.47
1:B:133:ASN:O	1:B:141:THR:OG1	2.30	0.47
1:B:135:ASP:OD1	1:B:135:ASP:N	2.45	0.47
2:D:20:LEU:CD1	2:D:32:SER:HB2	2.44	0.47
1:B:16:ARG:HG3	1:B:164:ASP:OD1	2.14	0.47
2:C:46:GLU:HG2	2:C:47:ALA:N	2.30	0.47
1:A:189:SER:O	1:A:191:ILE:HG22	2.15	0.47
1:B:186:ILE:HG12	1:B:187:ASP:H	1.80	0.47
2:D:48:HIS:CE1	2:D:129:VAL:HG23	2.50	0.47
1:A:14:ASP:OD2	1:A:15:LYS:HE3	2.06	0.46
1:A:16:ARG:NH1	1:A:98:PHE:CB	2.78	0.46
1:A:34:TRP:O	1:A:54:PHE:HB2	2.14	0.46
2:C:68:VAL:HB	2:C:82:VAL:HG11	1.97	0.46
1:A:97:ARG:NH1	1:A:97:ARG:CG	2.78	0.46
2:C:41:TYR:HE1	2:C:47:ALA:HB2	1.80	0.46
1:B:107:VAL:O	1:B:115:THR:HG23	2.16	0.46
1:A:7:VAL:HG22	1:A:173:GLN:HB3	1.98	0.46
1:B:20:LEU:HD21	1:B:29:ILE:HA	1.97	0.46
1:A:177:THR:O	1:A:198:ASN:ND2	2.48	0.46
1:B:20:LEU:O	1:B:59:GLY:N	2.45	0.45
1:B:25:ASN:OD1	1:B:28:GLN:NE2	2.49	0.45
1:B:87:THR:HG22	1:B:124:GLN:HE21	1.81	0.45
1:A:16:ARG:NH1	1:A:102:GLY:HA2	2.32	0.45
2:C:127:TYR:CZ	2:C:143:HIS:CD2	3.05	0.45
2:C:24:ALA:O	2:C:25:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:19:GLU:O	2:C:20:LEU:HD22	2.17	0.45
2:C:50:LEU:HD12	2:C:51:GLN:N	2.32	0.44
2:D:82:VAL:HG21	2:D:94:PHE:HD2	1.82	0.44
1:A:16:ARG:CG	1:A:103:HIS:CE1	2.98	0.44
1:A:149:LEU:HB3	1:A:150:GLY:H	1.47	0.44
1:A:84:ILE:HD12	1:A:114:VAL:HG13	1.98	0.44
2:D:25:ASN:CG	2:D:26:ARG:H	2.26	0.44
2:D:62:ASN:HA	2:D:161:GLN:HE22	1.82	0.44
1:A:34:TRP:CH2	1:A:167:THR:HG22	2.52	0.44
1:B:86:THR:OG1	1:B:87:THR:N	2.49	0.44
1:A:126:SER:HA	1:A:143:HIS:O	2.18	0.44
2:C:124:GLN:HG2	2:C:146:ASP:OD2	2.18	0.44
1:A:86:THR:OG1	1:A:87:THR:N	2.51	0.43
1:A:95:ILE:HG13	1:A:108:THR:HG21	1.99	0.43
1:A:188:GLN:O	1:A:189:SER:OG	2.34	0.43
2:D:151:GLU:H	2:D:151:GLU:HG2	1.47	0.43
1:B:39:LYS:NZ	1:B:49:GLU:OE1	2.51	0.43
1:A:16:ARG:HH12	1:A:98:PHE:CB	2.30	0.43
1:A:109:ASP:HB3	1:A:114:VAL:CG2	2.48	0.43
1:A:16:ARG:NH2	1:A:98:PHE:CD2	2.86	0.43
2:C:26:ARG:HG3	2:C:28:GLN:CB	2.46	0.43
1:A:16:ARG:HH12	1:A:98:PHE:HB2	1.83	0.43
2:C:70:VAL:HG11	2:C:127:TYR:CB	2.45	0.43
2:C:78:THR:C	2:C:80:THR:N	2.75	0.43
1:B:135:ASP:OD1	1:B:139:ALA:N	2.52	0.43
2:D:4:THR:HG23	2:D:41:TYR:H	1.84	0.43
2:D:152:ILE:HD12	2:D:152:ILE:C	2.44	0.42
2:D:48:HIS:HE1	2:D:129:VAL:HG23	1.83	0.42
1:B:-3:GLN:HG3	1:B:-2:LYS:N	2.34	0.42
2:D:64:TRP:NE1	2:D:161:GLN:HE21	2.15	0.42
1:B:107:VAL:H	1:B:115:THR:HG23	1.84	0.42
1:A:53:ASP:O	1:A:66:ALA:HA	2.20	0.42
1:B:198:ASN:OD1	1:B:200:VAL:HG23	2.19	0.42
1:A:16:ARG:NH2	1:A:98:PHE:HD2	2.18	0.42
1:A:176:TYR:CD1	1:A:198:ASN:ND2	2.88	0.42
1:B:104:LEU:HD21	1:B:121:VAL:CG1	2.49	0.42
1:B:20:LEU:HD11	1:B:32:SER:HB2	2.01	0.41
1:B:164:ASP:O	1:B:165:LYS:HG2	2.20	0.41
2:C:127:TYR:OH	2:C:143:HIS:CD2	2.72	0.41
2:D:109:ASP:O	2:D:111:ALA:N	2.53	0.41
1:A:68:VAL:HG12	1:A:92:ASN:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HH11	1:A:97:ARG:CG	2.24	0.41
1:A:7:VAL:HG11	1:A:38:PHE:CE1	2.55	0.41
1:A:136:GLU:O	1:A:138:GLY:N	2.53	0.41
1:A:202:GLN:HG3	1:A:203:GLU:N	2.35	0.41
2:C:142:ARG:H	2:C:142:ARG:HG3	1.62	0.41
1:B:112:GLY:O	1:B:114:VAL:HG23	2.21	0.41
1:A:14:ASP:O	1:A:16:ARG:N	2.54	0.41
1:A:87:THR:HG21	1:A:126:SER:OG	2.21	0.41
2:C:90:VAL:HG23	2:C:110:THR:OG1	2.21	0.41
1:B:151:GLU:HG3	1:B:154:THR:HG22	2.02	0.41
1:A:148:ASN:HB3	1:A:149:LEU:H	1.63	0.41
1:B:24:ALA:HB1	1:B:28:GLN:HB2	2.04	0.40
1:B:61:VAL:HG12	1:B:62:ASN:N	2.36	0.40
1:A:207:ILE:HD12	1:A:207:ILE:HA	1.92	0.40
2:D:17:LEU:HA	2:D:18:PRO:HD3	1.86	0.40
2:D:78:THR:O	2:D:80:THR:N	2.54	0.40
2:D:81:ARG:HH21	2:D:142:ARG:CZ	2.34	0.40
1:B:194:GLY:O	1:B:201:ARG:HA	2.21	0.40
1:A:55:ALA:O	1:A:64:TRP:HA	2.22	0.40
2:C:84:ILE:HB	2:C:113:ASN:HB2	2.04	0.40
2:C:128:ASN:CB	2:C:140:PRO:HB2	2.51	0.40
1:A:136:GLU:C	1:A:138:GLY:N	2.78	0.40
2:C:114:VAL:HG22	2:C:115:THR:N	2.37	0.40
2:D:80:THR:O	2:D:92:ASN:HB3	2.21	0.40
1:A:120:GLN:H	1:A:120:GLN:HG2	1.69	0.40
2:D:123:VAL:O	2:D:124:GLN:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:NH1	2:D:112:GLY:N[1_454]	2.11	0.09

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	197/333 (59%)	160 (81%)	18 (9%)	19 (10%)	0	2
1	B	216/333 (65%)	196 (91%)	13 (6%)	7 (3%)	3	16
2	C	166/177 (94%)	137 (82%)	17 (10%)	12 (7%)	1	4
2	D	169/177 (96%)	137 (81%)	21 (12%)	11 (6%)	1	5
All	All	748/1020 (73%)	630 (84%)	69 (9%)	49 (7%)	1	5

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	163	SER
1	A	18	PRO
1	A	58	PRO
1	A	116	SER
1	A	137	ALA
2	C	25	ASN
2	C	26	ARG
2	C	80	THR
2	C	126	SER
2	C	127	TYR
2	D	5	THR
2	D	76	ASP
2	D	141	THR
1	B	115	THR
1	B	141	THR
1	B	188	GLN
1	A	11	ALA
1	A	13	LEU
1	A	16	ARG
1	A	21	PRO
1	A	61	VAL
1	A	100	ASN
2	C	130	VAL
2	C	142	ARG
2	D	84	ILE
2	D	110	THR
1	A	15	LYS
1	A	64	TRP
1	A	136	GLU
1	A	149	LEU

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Mol	Chain	Res	Type
2	C	19	GLU
2	C	139	ALA
2	D	79	ALA
2	D	139	ALA
1	B	156	LYS
1	B	189	SER
1	A	106	SER
1	A	190	GLY
2	C	134	PRO
2	D	133	ASN
1	B	165	LYS
1	A	180	TYR
2	C	132	ALA
2	C	143	HIS
1	A	201	ARG
2	D	124	GLN
2	D	134	PRO
2	D	146	ASP
1	A	17	LEU

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	162/262 (62%)	162 (100%)	0	100	100
1	B	178/262 (68%)	178 (100%)	0	100	100
2	C	138/143 (96%)	138 (100%)	0	100	100
2	D	138/143 (96%)	138 (100%)	0	100	100
All	All	616/810 (76%)	616 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	ASN
1	B	103	HIS
1	A	28	GLN
1	A	69	ASN
1	A	148	ASN
2	C	69	ASN
2	C	128	ASN
2	C	133	ASN
2	D	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	DAL	D	11	1,2	3,4,5	0.72	0	2,4,6	1.07	0
2	DAL	C	11	1,2	3,4,5	0.53	0	2,4,6	0.83	0

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	DAL	D	11	1,2	-	0/1/2/4	-
2	DAL	C	11	1,2	-	0/1/2/4	-

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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	201/333 (60%)	0.26	14 (6%) 22 11	38, 85, 124, 143	0
1	B	218/333 (65%)	-0.21	0 100 100	34, 59, 87, 110	0
2	C	170/177 (96%)	0.09	3 (1%) 67 43	40, 66, 130, 162	0
2	D	171/177 (96%)	0.15	2 (1%) 76 54	39, 76, 132, 177	0
All	All	760/1020 (74%)	0.06	19 (2%) 58 34	34, 69, 121, 177	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	ALA	4.2
2	D	137	ALA	2.8
2	C	20	LEU	2.7
1	A	207	ILE	2.6
1	A	112	GLY	2.6
2	D	125	ILE	2.5
1	A	118	ALA	2.4
1	A	104	LEU	2.4
1	A	10	ALA	2.4
1	A	55	ALA	2.3
1	A	107	VAL	2.2
1	A	149	LEU	2.2
1	A	169	LYS	2.2
1	A	23	GLY	2.1
1	A	137	ALA	2.1
1	A	151	GLU	2.1
2	C	134	PRO	2.1
2	C	27	ALA	2.0
1	A	117	PRO	2.0

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
2	DAL	C	11	5/6	0.91	0.12	41,42,45,45	0
2	DAL	D	11	5/6	0.92	0.08	43,46,49,53	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.