



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:14 PM UTC

PDB ID : 3FMT / pdb_00003fmt
Title : Crystal structure of SeqA bound to DNA
Authors : Chung, Y.S.; Brendler, T.; Austin, S.; Guarne, A.
Deposited on : 2008-12-22
Resolution : 2.98 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

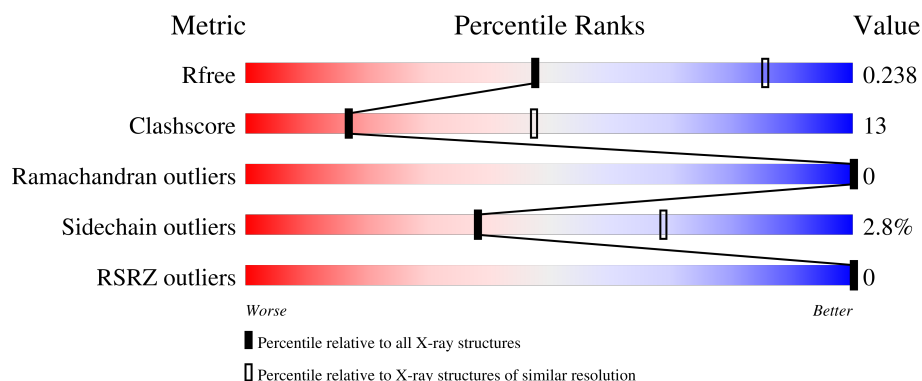
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

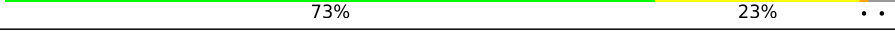
The reported resolution of this entry is 2.98 Å.

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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	162	
1	B	162	
1	E	162	
1	F	162	
2	C	22	

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Mol	Chain	Length	Quality of chain
2	G	22	 77% 23%
3	D	22	 50% 45% 5%
3	H	22	 45% 50% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6963 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 Protein seqA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1297	816	228	244	9			
1	B	157	Total	C	N	O	S	0	1	0
			1274	804	225	236	9			
1	E	162	Total	C	N	O	S	0	0	0
			1297	816	228	244	9			
1	F	157	Total	C	N	O	S	0	1	0
			1274	804	225	236	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ARG	ALA	engineered mutation	UNP P0AFY8
B	25	ARG	ALA	engineered mutation	UNP P0AFY8
E	25	ARG	ALA	engineered mutation	UNP P0AFY8
F	25	ARG	ALA	engineered mutation	UNP P0AFY8

- Molecule 2 is a DNA chain called 5'-D(*GP*AP*GP*TP*CP*GP*(6MA)P*TP*CP*GP*GP*CP*GP*GP*GP*(6MA)P*TP*CP*CP*TP*TP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	P	0	0	0
			454	217	85	131	21			
2	G	22	Total	C	N	O	P	0	0	0
			454	217	85	131	21			

- Molecule 3 is a DNA chain called 5'-D(*TP*CP*TP*AP*AP*GP*GP*AP*TP*CP*CP*CP*GP*CP*CP*GP*AP*TP*CP*GP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	21	Total	C	N	O	P	0	0	0
			425	203	79	123	20			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	21	Total	C	N	O	P	0	0	0
			425	203	79	123	20			

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		
4	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	B	4	Total	O	0	0
			4	4		
5	C	5	Total	O	0	0
			5	5		
5	D	4	Total	O	0	0
			4	4		

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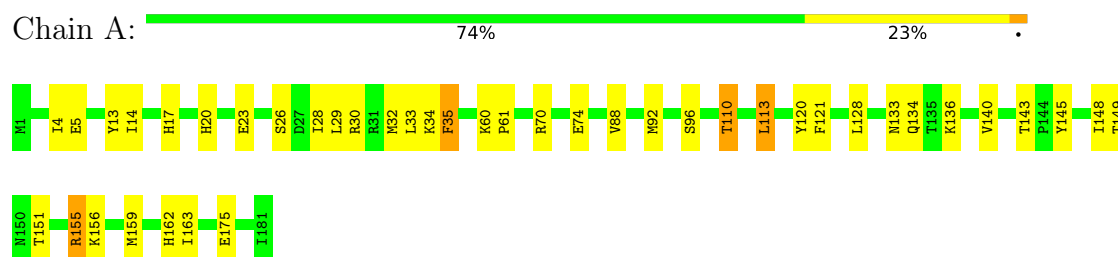
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	3	Total 3	O 3	0	0
5	F	7	Total 7	O 7	0	0
5	G	3	Total 3	O 3	0	0
5	H	3	Total 3	O 3	0	0

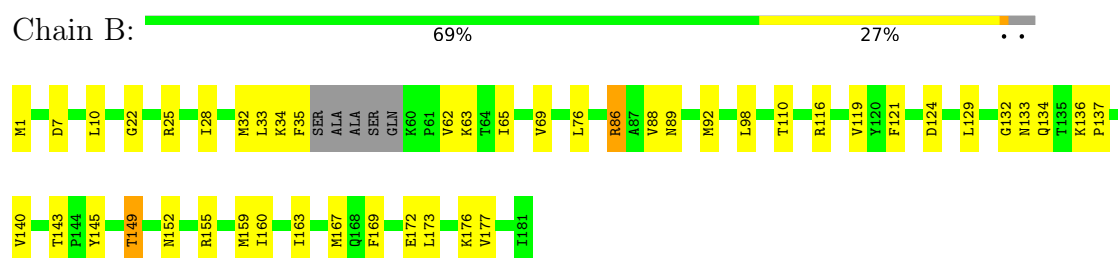
3 Residue-property plots

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.

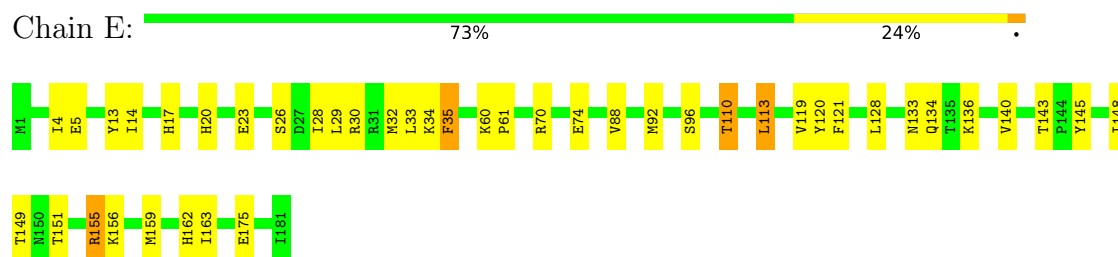
• Molecule 1: Protein seqA



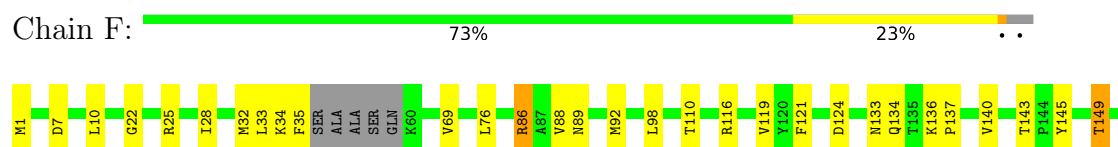
• Molecule 1: Protein seqA



• Molecule 1: Protein seqA



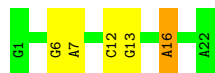
• Molecule 1: Protein seqA





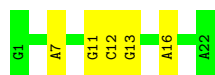
- Molecule 2: 5'-D(*GP*AP*GP*TP*CP*GP*(6MA)P*TP*CP*GP*GP*CP*GP*GP*GP*(6MA)P*TP*CP*CP*TP*TP*A)-3'

Chain C: 77% 18% 5%



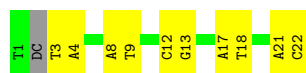
- Molecule 2: 5'-D(*GP*AP*GP*TP*CP*GP*(6MA)P*TP*CP*GP*GP*CP*GP*GP*GP*(6MA)P*TP*CP*CP*TP*TP*A)-3'

Chain G: 77% 23%



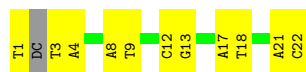
- Molecule 3: 5'-D(*TP*CP*TP*AP*AP*GP*GP*AP*TP*CP*CP*CP*GP*CP*CP*GP*AP*TP*CP*GP*AP*C)-3'

Chain D: 50% 45% 5%



- Molecule 3: 5'-D(*TP*CP*TP*AP*AP*GP*GP*AP*TP*CP*CP*CP*GP*CP*CP*GP*AP*TP*CP*GP*AP*C)-3'

Chain H: 45% 50% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	121.84Å 121.84Å 279.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.17 – 2.98 35.17 – 2.98	Depositor EDS
% Data completeness (in resolution range)	96.3 (35.17-2.98) 96.3 (35.17-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.218 , 0.245 0.213 , 0.238	Depositor DCC
R_{free} test set	1533 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6963	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: MPD, 6MA

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	0/1319	0.68	0/1774
1	B	0.32	0/1298	0.70	0/1743
1	E	0.29	0/1319	0.68	0/1774
1	F	0.32	0/1298	0.70	0/1743
2	C	0.21	0/457	0.70	0/700
2	G	0.22	0/457	0.70	0/700
3	D	0.24	0/475	0.79	0/728
3	H	0.23	0/475	0.79	0/728
All	All	0.29	0/7098	0.71	0/9890

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	1297	0	1320	41	0
1	B	1274	0	1304	42	0
1	E	1297	0	1320	41	0
1	F	1274	0	1304	40	0
2	C	454	0	253	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	454	0	253	5	0
3	D	425	0	238	5	0
3	H	425	0	238	6	0
4	A	16	0	28	4	0
4	E	16	0	28	4	0
5	A	2	0	0	0	0
5	B	4	0	0	0	0
5	C	5	0	0	0	0
5	D	4	0	0	0	0
5	E	3	0	0	0	0
5	F	7	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	0	0
All	All	6963	0	6286	168	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 13.

All (168) 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:F:143:THR:HG22	1:F:145:TYR:H	1.22	1.04
1:B:143:THR:HG22	1:B:145:TYR:H	1.22	1.01
1:F:86:ARG:HH11	1:F:86:ARG:HG2	1.35	0.91
1:B:86:ARG:HH11	1:B:86:ARG:HG2	1.35	0.87
1:F:86:ARG:HH11	1:F:86:ARG:CG	1.94	0.81
3:H:17:DA:H2''	3:H:18:DT:H72	1.62	0.80
1:B:86:ARG:HH11	1:B:86:ARG:CG	1.94	0.80
1:A:143:THR:HG22	1:A:145:TYR:H	1.46	0.80
1:E:143:THR:HG22	1:E:145:TYR:H	1.46	0.79
1:B:140:VAL:O	1:B:143:THR:HB	1.83	0.78
1:F:140:VAL:O	1:F:143:THR:HB	1.84	0.76
3:D:8:DA:H2''	3:D:9:DT:H72	1.70	0.74
1:A:28:ILE:HG22	1:A:32:MET:HE3	1.72	0.71
1:A:14:ILE:HA	1:A:32:MET:HE1	1.72	0.71
1:E:14:ILE:HA	1:E:32:MET:HE1	1.72	0.71
1:E:28:ILE:HG22	1:E:32:MET:HE3	1.72	0.70
1:B:86:ARG:HG2	1:B:86:ARG:NH1	2.03	0.70
1:E:140:VAL:HG23	1:E:143:THR:HB	1.74	0.70
1:A:140:VAL:HG23	1:A:143:THR:HB	1.73	0.68
1:B:143:THR:HG22	1:B:145:TYR:N	2.04	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:THR:HG22	1:F:145:TYR:N	2.03	0.67
1:F:86:ARG:HG2	1:F:86:ARG:NH1	2.02	0.67
1:F:136:LYS:O	1:F:149:THR:HB	1.95	0.66
1:B:136:LYS:O	1:B:149:THR:HB	1.94	0.66
1:B:86:ARG:H	1:B:89:ASN:HD22	1.45	0.65
1:F:98:LEU:HB3	1:F:167:MET:HE1	1.79	0.65
3:H:8:DA:H2''	3:H:9:DT:H71	1.80	0.64
1:B:98:LEU:HB3	1:B:167:MET:HE1	1.78	0.64
1:F:86:ARG:H	1:F:89:ASN:HD22	1.45	0.64
1:E:113:LEU:HD22	1:E:120:TYR:HD2	1.65	0.61
2:C:12:DC:H2''	2:C:13:DG:C8	2.36	0.61
2:G:12:DC:H2''	2:G:13:DG:C8	2.36	0.60
1:A:113:LEU:HD22	1:A:120:TYR:HD2	1.65	0.60
1:A:5:GLU:HB3	1:B:1:MET:HE3	1.84	0.60
1:A:110:THR:HG23	1:A:121:PHE:HB2	1.84	0.60
1:E:110:THR:HG23	1:E:121:PHE:HB2	1.84	0.60
1:E:35:PHE:C	1:E:35:PHE:CD1	2.80	0.59
1:E:5:GLU:HB3	1:F:1:MET:HE3	1.83	0.59
1:A:35:PHE:C	1:A:35:PHE:CD1	2.80	0.59
1:A:155:ARG:HH11	1:A:155:ARG:HB2	1.68	0.58
1:E:155:ARG:HH11	1:E:155:ARG:HB2	1.68	0.58
1:E:70:ARG:O	1:E:74:GLU:HG2	2.04	0.57
3:D:17:DA:H2''	3:D:18:DT:H71	1.86	0.57
1:E:17:HIS:HB2	1:E:32:MET:HE2	1.87	0.57
1:F:76:LEU:HD11	1:F:177:VAL:HG22	1.86	0.57
1:A:70:ARG:O	1:A:74:GLU:HG2	2.04	0.57
1:B:76:LEU:HD11	1:B:177:VAL:HG22	1.86	0.56
1:E:5:GLU:HB3	1:F:1:MET:CE	2.36	0.56
1:F:69:VAL:HG13	1:F:173:LEU:HD22	1.87	0.56
1:A:17:HIS:HB2	1:A:32:MET:HE2	1.87	0.56
1:E:136:LYS:O	1:E:149:THR:HB	2.06	0.56
1:A:136:LYS:O	1:A:149:THR:HB	2.06	0.55
1:B:33:LEU:O	1:B:34:LYS:HB2	2.06	0.55
1:B:69:VAL:HG13	1:B:173:LEU:HD22	1.87	0.55
1:A:34:LYS:HB2	4:A:183:MPD:H53	1.87	0.55
1:F:163:ILE:HG22	1:F:167:MET:HE2	1.89	0.55
1:B:163:ILE:HG22	1:B:167:MET:HE2	1.89	0.55
1:E:88:VAL:O	1:E:92:MET:HG2	2.06	0.55
1:A:30:ARG:NH2	4:A:183:MPD:H11	2.22	0.55
1:A:88:VAL:O	1:A:92:MET:HG2	2.07	0.55
1:F:98:LEU:HD22	1:F:167:MET:HE1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:LYS:HA	1:E:159:MET:HE3	1.89	0.54
1:F:33:LEU:O	1:F:34:LYS:HB2	2.06	0.54
1:B:98:LEU:HD22	1:B:167:MET:HE1	1.90	0.54
1:A:5:GLU:HB3	1:B:1:MET:CE	2.36	0.54
1:A:17:HIS:CB	1:A:32:MET:HE2	2.38	0.54
1:A:156:LYS:HA	1:A:159:MET:HE3	1.89	0.53
1:A:60:LYS:HB3	1:A:61:PRO:HD2	1.90	0.53
1:E:17:HIS:CB	1:E:32:MET:HE2	2.38	0.53
1:A:34:LYS:HB2	4:A:183:MPD:C5	2.39	0.53
1:A:128:LEU:HD13	1:A:148:ILE:HG23	1.91	0.53
1:E:60:LYS:HB3	1:E:61:PRO:HD2	1.90	0.53
1:F:22:GLY:HA3	1:F:119:VAL:CG2	2.39	0.52
1:B:22:GLY:HA3	1:B:119:VAL:CG2	2.40	0.52
1:F:116[B]:ARG:HD3	2:G:13:DG:H5'	1.91	0.52
3:H:12:DC:H2''	3:H:13:DG:C8	2.45	0.52
1:E:32:MET:HA	1:E:35:PHE:CD1	2.45	0.51
1:A:32:MET:HA	1:A:35:PHE:CD1	2.45	0.51
1:E:128:LEU:HD13	1:E:148:ILE:HG23	1.91	0.51
1:B:167:MET:HE3	1:B:169:PHE:HE2	1.76	0.51
3:D:12:DC:H2''	3:D:13:DG:C8	2.45	0.51
1:E:30:ARG:NH2	4:E:183:MPD:H11	2.25	0.51
1:E:34:LYS:HB2	4:E:183:MPD:C5	2.41	0.50
1:F:167:MET:HE3	1:F:169:PHE:HE2	1.76	0.50
1:A:32:MET:HA	1:A:35:PHE:CE1	2.47	0.50
1:E:34:LYS:HB2	4:E:183:MPD:H53	1.94	0.49
1:E:20:HIS:NE2	1:E:23:GLU:HB3	2.28	0.49
1:E:30:ARG:HH11	1:F:7:ASP:CG	2.20	0.49
3:H:3:DT:H2''	3:H:4:DA:C8	2.48	0.49
1:B:76:LEU:HD13	4:E:182:MPD:H11	1.94	0.49
3:D:3:DT:H2''	3:D:4:DA:C8	2.48	0.49
1:A:30:ARG:HH11	1:B:7:ASP:CG	2.21	0.48
1:A:20:HIS:NE2	1:A:23:GLU:HB3	2.28	0.48
1:A:33:LEU:HD12	1:B:10:LEU:HD11	1.95	0.48
3:D:21:DA:H2''	3:D:22:DC:H5''	1.96	0.48
1:E:32:MET:HA	1:E:35:PHE:CE1	2.47	0.48
1:F:110:THR:HG23	1:F:121:PHE:CG	2.48	0.48
1:A:113:LEU:HD13	1:A:121:PHE:HE1	1.79	0.48
1:E:33:LEU:HD12	1:F:10:LEU:HD11	1.95	0.48
1:F:124:ASP:OD2	1:F:124:ASP:C	2.56	0.48
1:F:116[B]:ARG:HD3	2:G:13:DG:C5'	2.44	0.47
1:B:110:THR:HG23	1:B:121:PHE:CG	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ARG:HH11	1:B:86:ARG:CB	2.28	0.47
1:E:113:LEU:HD13	1:E:121:PHE:HE1	1.79	0.47
1:B:88:VAL:O	1:B:92:MET:HG2	2.15	0.47
3:H:21:DA:H2''	3:H:22:DC:H5''	1.96	0.47
1:A:4:ILE:HB	1:B:25:ARG:HG3	1.97	0.47
1:F:116[B]:ARG:NH1	2:G:11:DG:H21	2.12	0.47
1:E:28:ILE:CG2	1:E:32:MET:HE3	2.44	0.46
1:B:124:ASP:OD2	1:B:124:ASP:C	2.57	0.46
1:E:13:TYR:CE1	1:E:17:HIS:HE1	2.34	0.46
1:E:159:MET:O	1:E:163:ILE:HG13	2.15	0.46
1:F:86:ARG:HH11	1:F:86:ARG:CB	2.28	0.46
1:F:98:LEU:HD22	1:F:167:MET:CE	2.46	0.46
1:F:88:VAL:O	1:F:92:MET:HG2	2.15	0.46
4:A:182:MPD:H11	1:F:76:LEU:HD13	1.98	0.46
1:E:4:ILE:HB	1:F:25:ARG:HG3	1.96	0.46
1:E:113:LEU:HG	1:E:162:HIS:CD2	2.51	0.46
1:A:159:MET:O	1:A:163:ILE:HG13	2.15	0.46
1:B:159:MET:O	1:B:163:ILE:HG13	2.16	0.46
1:A:13:TYR:CE1	1:A:17:HIS:HE1	2.34	0.45
1:A:28:ILE:CG2	1:A:32:MET:HE3	2.44	0.45
1:B:116[A]:ARG:HD2	2:C:13:DG:H5'	1.99	0.45
1:A:113:LEU:HG	1:A:162:HIS:CD2	2.51	0.45
1:F:28:ILE:O	1:F:32:MET:HG3	2.17	0.45
1:B:98:LEU:HD22	1:B:167:MET:CE	2.46	0.45
1:F:159:MET:O	1:F:163:ILE:HG13	2.17	0.44
1:B:28:ILE:O	1:B:32:MET:HG3	2.17	0.44
1:A:17:HIS:CG	1:A:32:MET:HE2	2.53	0.43
1:B:136:LYS:N	1:B:137:PRO:HD3	2.33	0.43
1:F:116[A]:ARG:HD2	2:G:13:DG:H5'	1.99	0.43
1:F:133:ASN:O	1:F:134:GLN:HB2	2.18	0.43
1:F:136:LYS:N	1:F:137:PRO:HD3	2.33	0.43
1:A:133:ASN:O	1:A:134:GLN:HB2	2.19	0.43
1:F:22:GLY:HA3	1:F:119:VAL:HG21	2.01	0.43
1:B:35:PHE:CD2	1:B:35:PHE:C	2.97	0.43
1:B:155:ARG:O	1:B:159:MET:HG3	2.19	0.42
1:F:155:ARG:O	1:F:159:MET:HG3	2.20	0.42
1:B:133:ASN:O	1:B:134:GLN:HB2	2.18	0.42
1:F:35:PHE:CD2	1:F:35:PHE:C	2.97	0.42
3:H:1:DT:H6	3:H:1:DT:H2'	1.64	0.42
1:E:17:HIS:CG	1:E:32:MET:HE2	2.54	0.42
1:A:155:ARG:HB2	1:A:155:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:OE1	1:A:175:GLU:HA	2.20	0.42
1:E:151:THR:OG1	1:E:156:LYS:HE3	2.20	0.42
1:E:133:ASN:O	1:E:134:GLN:HB2	2.19	0.41
1:A:20:HIS:CD2	1:A:20:HIS:C	2.98	0.41
1:A:151:THR:OG1	1:A:156:LYS:HE3	2.20	0.41
1:A:14:ILE:HD13	1:A:29:LEU:HD21	2.02	0.41
1:B:160:ILE:HD13	1:B:160:ILE:HA	1.95	0.41
1:B:22:GLY:HA3	1:B:119:VAL:HG21	2.01	0.41
1:B:65:ILE:O	1:B:69:VAL:HG23	2.20	0.41
1:B:172:GLU:O	1:B:176:LYS:HG3	2.21	0.41
1:E:29:LEU:HD23	1:E:29:LEU:HA	1.88	0.41
1:E:175:GLU:OE1	1:E:175:GLU:HA	2.20	0.41
1:A:140:VAL:O	1:A:143:THR:HB	2.21	0.41
1:F:172:GLU:O	1:F:176:LYS:HG3	2.20	0.41
1:A:29:LEU:HD23	1:A:29:LEU:HA	1.88	0.40
1:B:129:LEU:O	1:B:132:GLY:O	2.39	0.40
1:E:14:ILE:HD13	1:E:29:LEU:HD21	2.02	0.40
1:B:152:ASN:HA	2:C:6:DG:H2''	2.03	0.40
1:E:20:HIS:CD2	1:E:20:HIS:C	2.98	0.40
1:E:140:VAL:O	1:E:143:THR:HB	2.21	0.40
1:F:173:LEU:O	1:F:177:VAL:HG23	2.21	0.40
1:B:62:VAL:HG22	1:B:63:LYS:N	2.37	0.40
1:B:173:LEU:O	1:B:177:VAL:HG23	2.21	0.40
2:C:16:6MA:N7	2:C:16:6MA:C1	2.84	0.40
1:E:119:VAL:O	1:E:128:LEU:HD22	2.21	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	160/162 (99%)	155 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	154/162 (95%)	150 (97%)	4 (3%)	0	100	100
1	E	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
1	F	154/162 (95%)	150 (97%)	4 (3%)	0	100	100
All	All	628/648 (97%)	610 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	143/143 (100%)	137 (96%)	6 (4%)	26	59
1	B	141/143 (99%)	139 (99%)	2 (1%)	59	80
1	E	143/143 (100%)	137 (96%)	6 (4%)	26	59
1	F	141/143 (99%)	139 (99%)	2 (1%)	59	80
All	All	568/572 (99%)	552 (97%)	16 (3%)	38	69

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	SER
1	A	35	PHE
1	A	96	SER
1	A	110	THR
1	A	113	LEU
1	A	155	ARG
1	B	86	ARG
1	B	149	THR
1	E	26	SER
1	E	35	PHE
1	E	96	SER
1	E	110	THR
1	E	113	LEU

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Mol	Chain	Res	Type
1	E	155	ARG
1	F	86	ARG
1	F	149	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	89	ASN
1	B	89	ASN
1	B	104	GLN
1	E	89	ASN
1	F	89	ASN
1	F	104	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	6MA	G	7	2,3	21,24,25	1.03	1 (4%)	27,34,37	2.26	10 (37%)
2	6MA	G	16	2,3	21,24,25	1.03	1 (4%)	27,34,37	2.26	9 (33%)
2	6MA	C	7	2,3	21,24,25	1.02	1 (4%)	27,34,37	2.25	10 (37%)
2	6MA	C	16	2,3	21,24,25	1.03	2 (9%)	27,34,37	2.24	9 (33%)

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	6MA	G	7	2,3	-	0/9/23/24	0/3/3/3
2	6MA	G	16	2,3	-	0/9/23/24	0/3/3/3
2	6MA	C	7	2,3	-	0/9/23/24	0/3/3/3
2	6MA	C	16	2,3	-	0/9/23/24	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	7	6MA	C8-N7	2.14	1.35	1.31
2	C	7	6MA	C8-N7	2.06	1.35	1.31
2	C	16	6MA	C5-N7	-2.06	1.35	1.39
2	G	16	6MA	C8-N7	2.04	1.35	1.31
2	C	16	6MA	C8-N7	2.03	1.35	1.31

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	16	6MA	C5-C4-N3	-5.36	119.34	126.72
2	C	16	6MA	C5-C4-N3	-5.25	119.49	126.72
2	C	7	6MA	C5-C4-N3	-4.90	119.97	126.72
2	G	7	6MA	N3-C2-N1	-4.87	121.21	128.58
2	G	7	6MA	C5-C4-N3	-4.86	120.03	126.72
2	C	7	6MA	N3-C2-N1	-4.84	121.26	128.58
2	C	16	6MA	N3-C2-N1	-4.79	121.33	128.58
2	G	16	6MA	N3-C2-N1	-4.75	121.40	128.58
2	G	7	6MA	N9-C8-N7	-4.15	108.04	113.94
2	C	7	6MA	N9-C8-N7	-4.07	108.16	113.94
2	C	16	6MA	N9-C8-N7	-3.74	108.63	113.94
2	G	16	6MA	N9-C8-N7	-3.71	108.67	113.94
2	C	7	6MA	C4-C5-N7	-3.51	106.57	110.58
2	G	16	6MA	C2-N3-C4	3.46	120.28	111.83
2	G	7	6MA	C4-C5-N7	-3.44	106.65	110.58
2	C	16	6MA	C2-N3-C4	3.43	120.22	111.83
2	C	7	6MA	C2-N3-C4	3.31	119.92	111.83
2	G	16	6MA	C4-C5-N7	-3.31	106.80	110.58
2	G	7	6MA	C2-N3-C4	3.31	119.91	111.83
2	G	16	6MA	N3-C4-N9	3.29	132.76	127.17
2	C	7	6MA	C5-N7-C8	3.26	108.57	103.45
2	C	16	6MA	C4-C5-N7	-3.25	106.86	110.58
2	C	16	6MA	N3-C4-N9	3.25	132.69	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	7	6MA	C5-N7-C8	3.23	108.53	103.45
2	G	7	6MA	C4-N9-C8	3.11	109.00	105.74
2	C	16	6MA	C5-N7-C8	3.01	108.19	103.45
2	G	16	6MA	C5-N7-C8	3.01	108.18	103.45
2	C	7	6MA	C4-N9-C8	2.99	108.88	105.74
2	C	7	6MA	N3-C4-N9	2.97	132.21	127.17
2	G	7	6MA	N3-C4-N9	2.96	132.20	127.17
2	G	16	6MA	C4-C5-C6	2.95	119.23	116.78
2	C	16	6MA	C4-C5-C6	2.81	119.11	116.78
2	C	16	6MA	C4-N9-C8	2.62	108.49	105.74
2	G	16	6MA	C4-N9-C8	2.60	108.46	105.74
2	C	7	6MA	C4-C5-C6	2.29	118.68	116.78
2	G	7	6MA	C4-C5-C6	2.27	118.67	116.78
2	C	7	6MA	C6-C5-N7	2.13	134.75	132.43
2	G	7	6MA	C6-C5-N7	2.07	134.69	132.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	16	6MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
4	MPD	E	183	-	7,7,7	0.30	0	9,10,10	0.18	0
4	MPD	E	182	-	7,7,7	0.27	0	9,10,10	0.23	0
4	MPD	A	183	-	7,7,7	0.31	0	9,10,10	0.20	0
4	MPD	A	182	-	7,7,7	0.27	0	9,10,10	0.21	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
4	MPD	E	183	-	-	1/5/5/5	-
4	MPD	E	182	-	-	2/5/5/5	-
4	MPD	A	183	-	-	2/5/5/5	-
4	MPD	A	182	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	183	MPD	C2-C3-C4-C5
4	E	183	MPD	C2-C3-C4-C5
4	A	182	MPD	O2-C2-C3-C4
4	A	183	MPD	O2-C2-C3-C4
4	E	182	MPD	O2-C2-C3-C4
4	A	182	MPD	C2-C3-C4-O4
4	E	182	MPD	C2-C3-C4-O4
4	A	182	MPD	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	183	MPD	3	0
4	E	182	MPD	1	0
4	A	183	MPD	3	0
4	A	182	MPD	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 [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	162/162 (100%)	-1.04	0 100 100	40, 74, 120, 145	0
1	B	157/162 (96%)	-1.27	0 100 100	23, 52, 110, 154	1 (0%)
1	E	162/162 (100%)	-1.04	0 100 100	41, 75, 119, 145	0
1	F	157/162 (96%)	-1.26	0 100 100	23, 51, 111, 160	1 (0%)
2	C	20/22 (90%)	-1.62	0 100 100	39, 59, 94, 110	0
2	G	20/22 (90%)	-1.64	0 100 100	37, 59, 97, 111	0
3	D	21/22 (95%)	-1.54	0 100 100	39, 60, 96, 132	0
3	H	21/22 (95%)	-1.53	0 100 100	39, 59, 96, 133	0
All	All	720/736 (97%)	-1.20	0 100 100	23, 64, 117, 160	2 (0%)

There are no RSRZ outliers to report.

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	6MA	C	7	22/23	1.00	0.03	39,39,39,39	0
2	6MA	C	16	22/23	1.00	0.04	54,54,54,54	0
2	6MA	G	7	22/23	1.00	0.03	37,37,37,37	0
2	6MA	G	16	22/23	1.00	0.03	54,54,54,54	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
4	MPD	A	182	8/8	0.99	0.06	71,71,71,71	0
4	MPD	A	183	8/8	0.99	0.07	87,87,87,87	0
4	MPD	E	182	8/8	0.99	0.07	72,72,72,72	0
4	MPD	E	183	8/8	0.99	0.09	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.