



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:27 PM UTC

PDB ID : 4PAR / pdb_00004par
Title : The 5-Hydroxymethylcytosine-Specific Restriction Enzyme AbaSI in a Complex with Product-like DNA
Authors : Horton, J.R.; Cheng, X.
Deposited on : 2014-04-09
Resolution : 2.89 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

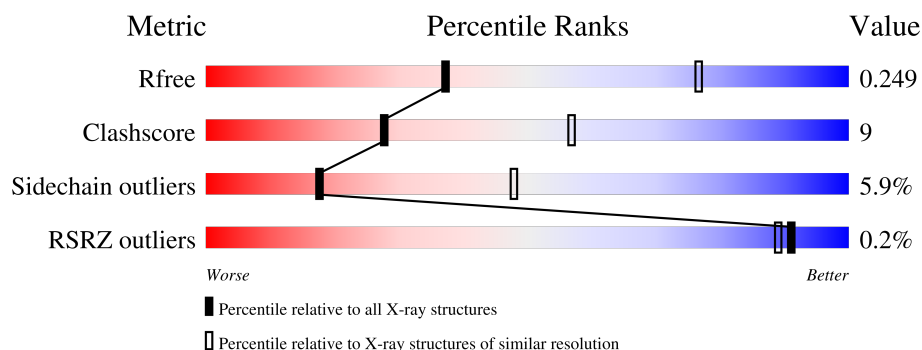
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	E	18	83% 17%
1	F	18	78% 22%
2	G	14	64% 36%
2	H	14	64% 36%
3	A	321	72% 24% ...
3	B	321	77% 20% ..

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Mol	Chain	Length	Quality of chain
3	C	321	69% 26% • •
3	D	321	71% 25% • •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11694 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 DNA chain called DNA 18-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	18	Total	C	N	O	P	0	0	0
			367	176	68	106	17			
1	F	18	Total	C	N	O	P	0	0	0
			367	176	68	106	17			

- Molecule 2 is a DNA chain called DNA 14-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	14	Total	C	N	O	P	0	0	0
			285	138	51	83	13			
2	H	14	Total	C	N	O	P	0	0	0
			285	138	51	83	13			

- Molecule 3 is a protein called Uncharacterized protein AbaSI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	313	Total	C	N	O	S	0	0	0
			2592	1653	445	488	6			
3	A	314	Total	C	N	O	S	0	0	0
			2601	1658	446	491	6			
3	C	314	Total	C	N	O	S	0	0	0
			2601	1659	447	489	6			
3	D	313	Total	C	N	O	S	0	0	0
			2592	1653	445	488	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	SER	CYS	engineered mutation	UNP B0VN39
B	309	SER	CYS	engineered mutation	UNP B0VN39
B	321	SER	CYS	engineered mutation	UNP B0VN39
A	2	SER	CYS	engineered mutation	UNP B0VN39
A	309	SER	CYS	engineered mutation	UNP B0VN39

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Chain	Residue	Modelled	Actual	Comment	Reference
A	321	SER	CYS	engineered mutation	UNP B0VN39
C	2	SER	CYS	engineered mutation	UNP B0VN39
C	309	SER	CYS	engineered mutation	UNP B0VN39
C	321	SER	CYS	engineered mutation	UNP B0VN39
D	2	SER	CYS	engineered mutation	UNP B0VN39
D	309	SER	CYS	engineered mutation	UNP B0VN39
D	321	SER	CYS	engineered mutation	UNP B0VN39

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	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: DNA 18-MER

Chain E:  83% 17%



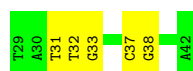
- Molecule 1: DNA 18-MER

Chain F:  78% 22%



- Molecule 2: DNA 14-MER

Chain G:  64% 36%



- Molecule 2: DNA 14-MER

Chain H:  64% 36%



- Molecule 3: Uncharacterized protein AbaSI

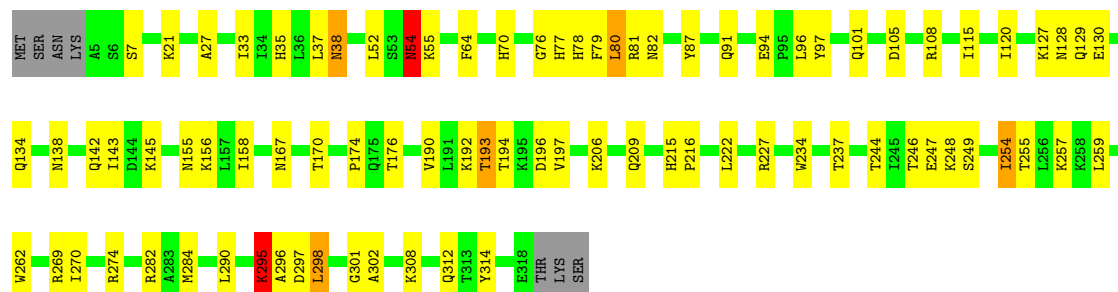
Chain B:  77% 20% ..





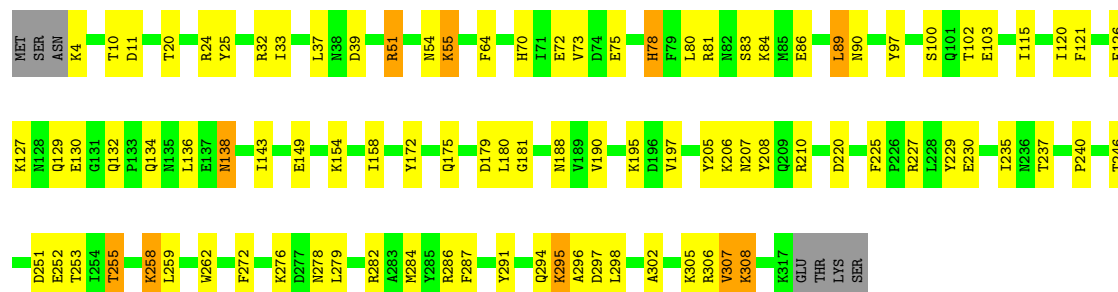
• Molecule 3: Uncharacterized protein AbaSI

Chain A: 72% 24% ...



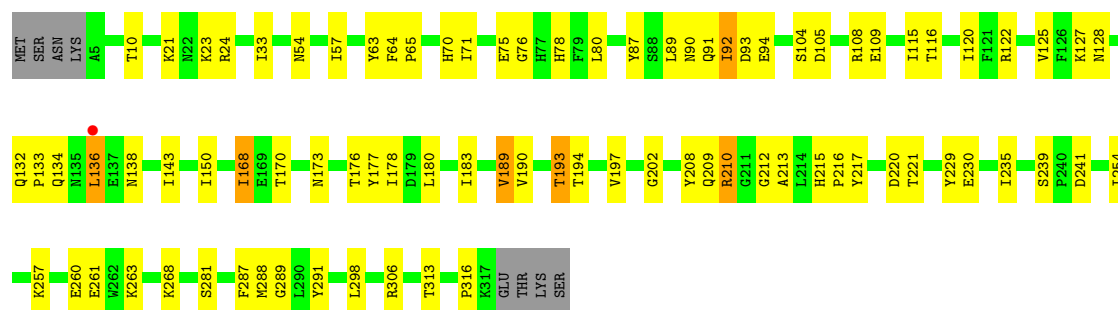
• Molecule 3: Uncharacterized protein AbaSI

Chain C: 69% 26% . .



• Molecule 3: Uncharacterized protein AbaSI

Chain D: 71% 25% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.83Å 144.70Å 105.03Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	34.90 – 2.89 34.90 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.0 (34.90-2.89) 90.7 (34.90-2.89)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1593)	Depositor
R, R_{free}	0.190 , 0.249 0.203 , 0.249	Depositor DCC
R_{free} test set	1791 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.647	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 56.7	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	0.95	EDS
Total number of atoms	11694	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.07% 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: 5HC, EDO

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	E	0.23	0/387	0.38	0/593
1	F	0.40	0/387	0.52	1/593 (0.2%)
2	G	0.23	0/319	0.41	0/491
2	H	0.21	0/319	0.41	0/491
3	A	0.45	0/2655	0.81	5/3583 (0.1%)
3	B	0.33	0/2646	0.77	2/3571 (0.1%)
3	C	0.36	0/2655	0.81	3/3582 (0.1%)
3	D	0.34	0/2646	0.81	4/3571 (0.1%)
All	All	0.36	0/12014	0.76	15/16475 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	132	GLN	CA-C-N	7.33	127.31	119.76
3	D	132	GLN	C-N-CA	7.33	127.31	119.76
3	A	54	ASN	N-CA-C	6.94	121.74	113.28
3	D	64	PHE	CA-C-N	6.93	126.17	118.97
3	D	64	PHE	C-N-CA	6.93	126.17	118.97
3	A	295	LYS	N-CA-C	6.08	118.37	108.76
3	A	64	PHE	CA-C-N	6.05	125.45	118.85
3	A	64	PHE	C-N-CA	6.05	125.45	118.85
3	C	295	LYS	N-CA-C	5.79	117.65	108.79
3	A	55	LYS	CB-CA-C	-5.40	104.48	109.83
1	F	13	DT	C2'-C3'-O3'	-5.23	103.65	111.50
3	C	64	PHE	CA-C-N	5.13	124.45	118.85
3	C	64	PHE	C-N-CA	5.13	124.45	118.85
3	B	173	ASN	CA-C-N	5.13	125.17	119.32
3	B	173	ASN	C-N-CA	5.13	125.17	119.32

There are no chirality outliers.

There are no planarity outliers.

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	E	367	0	206	2	0
1	F	367	0	206	2	0
2	G	285	0	161	5	0
2	H	285	0	161	6	0
3	A	2601	0	2596	66	0
3	B	2592	0	2590	33	0
3	C	2601	0	2603	56	0
3	D	2592	0	2590	46	0
4	C	4	0	6	0	0
All	All	11694	0	11119	205	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 9.

All (205) 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)
3:A:76:GLY:O	3:A:77:HIS:HB2	1.54	1.02
3:A:80:LEU:O	3:A:80:LEU:HD22	1.58	1.00
3:A:80:LEU:C	3:A:80:LEU:CD2	2.37	0.97
3:A:80:LEU:C	3:A:80:LEU:HD23	1.99	0.86
3:C:51:ARG:HH11	3:C:51:ARG:HG2	1.44	0.80
3:A:80:LEU:O	3:A:80:LEU:CD2	2.30	0.79
3:D:177:TYR:HB3	3:D:183:ILE:HD11	1.68	0.74
3:B:170:THR:HB	3:B:176:THR:HG21	1.69	0.74
3:A:248:LYS:HG2	3:A:249:SER:H	1.53	0.73
1:E:11:DA:OP1	3:B:282:ARG:NH1	2.23	0.71
3:A:80:LEU:HD22	3:A:80:LEU:C	2.10	0.70
3:D:57:ILE:HD12	3:D:104:SER:HB2	1.74	0.70
3:C:80:LEU:HD21	3:C:83:SER:HB2	1.75	0.69
3:A:127:LYS:HB3	3:A:134:GLN:HG3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:127:LYS:HG2	3:C:134:GLN:HG3	1.76	0.68
3:B:70:HIS:HB2	3:B:120:ILE:HG12	1.76	0.67
3:D:127:LYS:HG2	3:D:133:PRO:HA	1.76	0.67
3:D:183:ILE:HG23	3:D:189:VAL:HG11	1.78	0.66
3:A:80:LEU:CD2	3:A:81:ARG:O	2.44	0.66
3:A:78:HIS:O	3:A:80:LEU:N	2.29	0.65
3:A:222:LEU:HB3	3:A:269:ARG:HG2	1.77	0.65
3:C:252:GLU:HA	3:C:255:THR:HB	1.79	0.64
2:G:31:DT:H4'	3:C:207:ASN:HB2	1.77	0.64
3:A:254:ILE:HA	3:A:257:LYS:HG2	1.78	0.64
3:C:32:ARG:HD3	3:C:143:ILE:HD13	1.78	0.64
3:C:259:LEU:HD22	3:C:298:LEU:HD22	1.80	0.62
3:A:76:GLY:O	3:A:77:HIS:CB	2.35	0.62
3:B:260:GLU:HA	3:B:263:LYS:HE2	1.81	0.62
3:A:127:LYS:HG3	3:A:128:ASN:H	1.65	0.61
3:A:192:LYS:HG3	3:A:193:THR:HG22	1.83	0.61
3:C:51:ARG:HG2	3:C:51:ARG:NH1	2.13	0.60
3:A:290:LEU:HD23	3:A:308:LYS:HD3	1.83	0.60
3:D:70:HIS:HB2	3:D:120:ILE:HG12	1.83	0.60
3:C:259:LEU:HD13	3:C:298:LEU:HD13	1.83	0.60
3:B:290:LEU:HB3	3:B:308:LYS:HB2	1.84	0.60
2:G:32:DT:H2''	2:G:33:DG:C8	2.38	0.59
3:D:230:GLU:HG3	3:D:235:ILE:HG12	1.84	0.59
3:B:230:GLU:HG3	3:B:235:ILE:HG12	1.85	0.59
3:D:193:THR:OG1	3:D:194:THR:N	2.35	0.59
3:A:290:LEU:HB3	3:A:308:LYS:HB2	1.86	0.58
3:A:37:LEU:C	3:A:38:ASN:HD22	2.11	0.57
3:A:237:THR:HG1	3:A:246:THR:HG1	1.48	0.57
3:B:133:PRO:HG2	3:A:7:SER:HB2	1.85	0.57
3:C:237:THR:HG1	3:C:246:THR:HG1	1.50	0.57
3:A:33:ILE:HG12	3:A:143:ILE:HG23	1.86	0.56
3:D:94:GLU:O	3:D:122:ARG:NH2	2.39	0.56
3:A:76:GLY:N	3:A:97:TYR:OH	2.33	0.55
3:D:134:GLN:HB3	3:D:138:ASN:HB2	1.87	0.55
3:C:255:THR:HA	3:C:258:LYS:HD3	1.88	0.55
3:A:170:THR:HB	3:A:176:THR:HG21	1.88	0.55
3:D:168:ILE:HD12	3:D:168:ILE:H	1.72	0.55
3:D:173:ASN:O	3:D:176:THR:HG22	2.07	0.55
3:A:79:PHE:O	3:A:80:LEU:C	2.49	0.55
3:C:51:ARG:HG3	3:C:240:PRO:HA	1.88	0.54
3:C:180:LEU:N	3:C:181:GLY:HA2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:239:SER:OG	3:D:241:ASP:OD1	2.25	0.54
3:B:39:ASP:OD2	3:B:154:LYS:NZ	2.37	0.54
3:C:136:LEU:HG	3:D:10:THR:HG22	1.90	0.54
3:B:33:ILE:HD13	3:B:71:ILE:HD13	1.90	0.53
3:B:157:LEU:HB3	3:B:163:PHE:HB2	1.89	0.53
3:B:23:LYS:NZ	3:B:61:ASP:OD2	2.39	0.53
3:A:70:HIS:HB2	3:A:120:ILE:HG12	1.90	0.53
3:B:57:ILE:HD12	3:B:104:SER:HB3	1.92	0.52
3:C:78:HIS:O	3:C:80:LEU:N	2.43	0.52
3:D:176:THR:O	3:D:180:LEU:HG	2.10	0.52
3:C:70:HIS:HB2	3:C:120:ILE:HG12	1.91	0.52
2:H:39:DA:H5"	3:A:206:LYS:HD3	1.91	0.52
3:A:105:ASP:O	3:A:108:ARG:NH1	2.42	0.52
3:A:193:THR:OG1	3:A:194:THR:N	2.42	0.52
3:B:291:TYR:CE2	3:B:306:ARG:HB2	2.45	0.52
3:B:290:LEU:HD23	3:B:308:LYS:HD3	1.92	0.52
3:D:216:PRO:HB2	3:D:217:TYR:HD2	1.75	0.51
3:D:215:HIS:HD2	3:D:216:PRO:HD2	1.76	0.51
3:A:190:VAL:HG12	3:A:284:MET:HE2	1.93	0.50
3:C:33:ILE:HG12	3:C:143:ILE:HG23	1.92	0.50
3:C:272:PHE:CE2	3:C:287:PHE:HB2	2.46	0.50
3:A:79:PHE:O	3:A:80:LEU:O	2.29	0.50
3:C:134:GLN:HG2	3:C:138:ASN:ND2	2.27	0.50
1:F:8:DT:OP2	3:A:282:ARG:NH2	2.44	0.49
3:B:234:TRP:HH2	3:B:258:LYS:HE3	1.77	0.49
3:A:80:LEU:HD23	3:A:81:ARG:O	2.11	0.49
3:C:227:ARG:NH1	3:C:229:TYR:OH	2.43	0.49
3:C:86:GLU:OE2	3:C:100:SER:HB3	2.12	0.49
3:C:188:ASN:OD1	3:C:286:ARG:NH2	2.43	0.49
3:D:108:ARG:HD3	3:D:229:TYR:HB2	1.94	0.49
3:B:251:ASP:HB2	3:B:254:ILE:HD13	1.93	0.49
3:D:281:SER:O	3:D:281:SER:OG	2.27	0.49
3:A:297:ASP:OD1	3:A:298:LEU:N	2.46	0.49
3:C:134:GLN:HG2	3:C:138:ASN:HD21	1.78	0.49
3:D:221:THR:HG23	3:D:268:LYS:HE3	1.93	0.49
3:A:82:ASN:OD1	3:A:82:ASN:O	2.30	0.49
3:C:72:GLU:OE2	3:C:97:TYR:HD1	1.95	0.48
3:D:71:ILE:HD11	3:D:150:ILE:HD11	1.96	0.48
3:C:255:THR:HG23	3:C:298:LEU:HD11	1.95	0.48
3:D:178:ILE:HA	3:D:313:THR:HG21	1.95	0.48
3:A:35:HIS:O	3:A:38:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:247:GLU:HB3	3:A:302:ALA:HB3	1.96	0.48
3:B:215:HIS:CD2	3:B:218:LYS:HB2	2.49	0.48
3:B:237:THR:OG1	3:B:246:THR:HG22	2.14	0.48
3:C:259:LEU:HD11	3:C:296:ALA:HB1	1.96	0.48
3:D:288:MET:HA	3:D:288:MET:HE2	1.96	0.48
3:B:130:GLU:H	3:B:130:GLU:CD	2.23	0.47
3:C:307:VAL:HG22	3:C:308:LYS:N	2.29	0.47
1:E:10:DC:H2"	1:E:11:DA:C8	2.50	0.47
3:A:78:HIS:C	3:A:80:LEU:H	2.22	0.47
3:C:258:LYS:HG3	3:C:262:TRP:CZ3	2.49	0.47
1:F:14:DA:C2	2:H:30:DA:C2	3.03	0.47
3:B:208:TYR:CE2	3:B:210:ARG:HB2	2.50	0.47
3:A:215:HIS:HD2	3:A:216:PRO:HD2	1.80	0.47
3:D:89:LEU:HD12	3:D:90:ASN:H	1.80	0.47
3:D:91:GLN:HB2	3:D:94:GLU:CD	2.39	0.47
3:D:109:GLU:HA	3:D:229:TYR:CE2	2.50	0.47
3:C:11:ASP:OD1	3:D:24:ARG:NH2	2.47	0.47
3:D:63:TYR:CZ	3:D:65:PRO:HA	2.50	0.46
3:C:197:VAL:HG11	3:C:225:PHE:HE1	1.81	0.46
3:C:262:TRP:CE3	3:C:302:ALA:HB2	2.50	0.46
3:B:155:ASN:O	3:B:158:ILE:HG13	2.16	0.46
3:B:287:PHE:CZ	3:B:289:GLY:HA2	2.50	0.46
3:A:54:ASN:OD1	3:A:54:ASN:N	2.46	0.46
3:B:190:VAL:HG12	3:B:284:MET:HE3	1.98	0.46
3:D:23:LYS:HB3	3:D:75:GLU:CD	2.41	0.46
3:D:260:GLU:HA	3:D:263:LYS:HG2	1.97	0.46
3:A:234:TRP:HB2	3:A:248:LYS:O	2.15	0.46
3:C:172:TYR:CE1	3:C:284:MET:HE1	2.51	0.46
3:C:208:TYR:CZ	3:C:210:ARG:HB3	2.51	0.46
3:D:220:ASP:OD2	3:D:268:LYS:HE2	2.16	0.46
3:B:71:ILE:HD11	3:B:150:ILE:HD11	1.99	0.45
3:A:248:LYS:HG2	3:A:249:SER:N	2.26	0.45
3:A:142:GLN:HA	3:A:145:LYS:HE3	1.97	0.45
3:B:63:TYR:CZ	3:B:65:PRO:HA	2.51	0.45
3:A:155:ASN:O	3:A:158:ILE:HG13	2.17	0.45
3:A:37:LEU:O	3:A:38:ASN:ND2	2.33	0.45
3:A:52:LEU:HD22	3:A:94:GLU:HB3	1.99	0.45
3:B:228:LEU:HD23	3:B:228:LEU:HA	1.81	0.45
3:D:105:ASP:O	3:D:108:ARG:HG3	2.17	0.45
3:A:21:LYS:NZ	3:A:27:ALA:H	2.14	0.45
3:A:138:ASN:OD1	3:A:142:GLN:NE2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:208:TYR:CE2	3:D:213:ALA:HB2	2.52	0.45
3:C:230:GLU:HG3	3:C:235:ILE:HG12	1.99	0.45
2:G:32:DT:H2"	2:G:33:DG:H8	1.81	0.44
3:C:251:ASP:OD2	3:C:253:THR:OG1	2.30	0.44
3:C:154:LYS:O	3:C:158:ILE:HG23	2.17	0.44
3:A:130:GLU:H	3:A:130:GLU:CD	2.24	0.44
3:D:76:GLY:HA2	3:D:87:TYR:CZ	2.52	0.44
3:D:33:ILE:HG12	3:D:143:ILE:HG23	2.00	0.44
3:C:24:ARG:HB3	3:C:25:TYR:CD1	2.53	0.44
3:D:92:ILE:HG23	3:D:93:ASP:H	1.82	0.44
3:D:136:LEU:HD13	3:D:136:LEU:HA	1.71	0.44
2:G:33:DG:OP1	3:C:205:TYR:OH	2.20	0.44
3:C:175:GLN:NE2	3:C:179:ASP:OD1	2.49	0.43
3:C:225:PHE:HA	3:C:272:PHE:O	2.18	0.43
3:C:190:VAL:HG22	3:C:284:MET:HE2	2.00	0.43
3:C:39:ASP:OD2	3:C:154:LYS:NZ	2.49	0.43
3:C:121:PHE:CZ	3:C:149:GLU:HG2	2.53	0.43
3:B:248:LYS:HG2	3:B:249:SER:H	1.84	0.43
3:A:78:HIS:C	3:A:80:LEU:N	2.77	0.43
3:D:134:GLN:HB3	3:D:138:ASN:CB	2.49	0.43
3:A:76:GLY:HA3	3:A:87:TYR:CZ	2.54	0.43
3:A:81:ARG:HA	3:A:82:ASN:HA	1.46	0.43
3:A:101:GLN:N	3:A:101:GLN:OE1	2.49	0.43
3:D:254:ILE:HA	3:D:257:LYS:HG2	2.01	0.43
2:H:39:DA:H2"	2:H:40:DG:H8	1.84	0.42
3:C:24:ARG:HB3	3:C:25:TYR:HD1	1.85	0.42
3:D:210:ARG:HE	3:D:210:ARG:HB2	1.55	0.42
3:D:208:TYR:OH	3:D:212:GLY:O	2.36	0.42
3:C:75:GLU:HB2	3:C:126:PHE:CE2	2.54	0.42
2:H:38:DG:N2	3:A:209:GLN:OE1	2.46	0.42
3:A:262:TRP:CE3	3:A:302:ALA:HB2	2.54	0.42
3:C:278:ASN:OD1	3:C:279:LEU:N	2.53	0.42
3:C:295:LYS:HD3	3:C:297:ASP:OD2	2.20	0.42
3:A:259:LEU:HG	3:A:296:ALA:HB1	2.01	0.42
3:C:4:LYS:HE3	3:C:4:LYS:HB2	1.93	0.42
2:H:39:DA:H2"	2:H:40:DG:C8	2.55	0.42
3:D:202:GLY:HA2	3:D:316:PRO:HA	2.01	0.42
3:A:167:ASN:ND2	3:A:170:THR:OG1	2.52	0.42
3:C:89:LEU:HD22	3:C:90:ASN:H	1.84	0.42
3:B:288:MET:HA	3:B:288:MET:HE2	2.01	0.42
3:B:126:PHE:HB3	3:B:129:GLN:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:287:PHE:CZ	3:D:289:GLY:HA2	2.55	0.42
3:A:78:HIS:HE1	3:A:130:GLU:HB2	1.84	0.41
3:A:227:ARG:HH21	3:A:274:ARG:NH1	2.18	0.41
2:H:34:DT:H5"	3:C:20:THR:HG21	2.01	0.41
3:A:174:PRO:HG3	3:A:196:ASP:HB3	2.02	0.41
3:D:261:GLU:N	3:D:261:GLU:OE1	2.53	0.41
3:D:291:TYR:CE2	3:D:306:ARG:HB2	2.55	0.41
3:A:52:LEU:HB2	3:A:54:ASN:OD1	2.21	0.41
3:B:224:TRP:CE2	3:B:226:PRO:HB3	2.56	0.41
3:C:255:THR:O	3:C:258:LYS:HG2	2.20	0.41
3:C:278:ASN:OD1	3:C:278:ASN:C	2.63	0.41
3:A:312:GLN:NE2	3:A:314:TYR:OH	2.54	0.41
3:A:91:GLN:HB2	3:A:94:GLU:CD	2.46	0.41
3:A:297:ASP:HB3	3:A:301:GLY:HA2	2.03	0.41
3:D:21:LYS:HD3	3:D:21:LYS:HA	1.85	0.41
3:B:202:GLY:HA2	3:B:316:PRO:HA	2.03	0.41
3:B:215:HIS:ND1	3:B:216:PRO:HD2	2.36	0.41
2:G:37:DC:H2"	2:G:38:DG:C8	2.55	0.40
3:A:254:ILE:HG13	3:A:255:THR:N	2.35	0.40
3:A:295:LYS:HE2	3:A:295:LYS:HB2	1.69	0.40
3:C:195:LYS:HD3	3:C:206:LYS:O	2.21	0.40
3:C:291:TYR:CE2	3:C:306:ARG:HB2	2.56	0.40
3:B:101:GLN:HA	3:B:104:SER:HB2	2.02	0.40
3:A:237:THR:OG1	3:A:246:THR:OG1	2.27	0.40
3:C:54:ASN:O	3:C:55:LYS:HB2	2.21	0.40
3:C:129:GLN:HG2	3:C:130:GLU:H	1.85	0.40
3:D:177:TYR:O	3:D:313:THR:HG21	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	
3	A	289/296 (98%)	275 (95%)	14 (5%)	23	55
3	B	288/296 (97%)	275 (96%)	13 (4%)	24	58
3	C	289/296 (98%)	266 (92%)	23 (8%)	11	34
3	D	288/296 (97%)	270 (94%)	18 (6%)	16	45
All	All	1154/1184 (98%)	1086 (94%)	68 (6%)	18	48

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	55	LYS
3	B	92	ILE
3	B	115	ILE
3	B	129	GLN
3	B	130	GLU
3	B	132	GLN
3	B	134	GLN
3	B	148	GLU
3	B	197	VAL
3	B	207	ASN
3	B	209	GLN
3	B	232	LYS
3	B	288	MET
3	A	38	ASN
3	A	54	ASN
3	A	80	LEU
3	A	96	LEU
3	A	115	ILE
3	A	129	GLN
3	A	156	LYS
3	A	193	THR
3	A	197	VAL
3	A	244	THR
3	A	254	ILE
3	A	270	ILE
3	A	295	LYS
3	A	298	LEU
3	C	10	THR
3	C	37	LEU
3	C	51	ARG

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Mol	Chain	Res	Type
3	C	55	LYS
3	C	73	VAL
3	C	78	HIS
3	C	81	ARG
3	C	84	LYS
3	C	89	LEU
3	C	102	THR
3	C	103	GLU
3	C	115	ILE
3	C	132	GLN
3	C	138	ASN
3	C	220	ASP
3	C	255	THR
3	C	258	LYS
3	C	276	LYS
3	C	282	ARG
3	C	294	GLN
3	C	305	LYS
3	C	307	VAL
3	C	308	LYS
3	D	54	ASN
3	D	78	HIS
3	D	80	LEU
3	D	92	ILE
3	D	115	ILE
3	D	116	THR
3	D	125	VAL
3	D	128	ASN
3	D	136	LEU
3	D	168	ILE
3	D	170	THR
3	D	189	VAL
3	D	190	VAL
3	D	193	THR
3	D	197	VAL
3	D	209	GLN
3	D	210	ARG
3	D	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	B	82	ASN
3	B	138	ASN
3	B	199	ASN
3	A	167	ASN
3	A	175	GLN
3	A	312	GLN
3	C	135	ASN
3	C	155	ASN
3	C	267	GLN
3	C	294	GLN
3	D	167	ASN

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$
1	5HC	E	5	2,1	18,22,23	4.00	9 (50%)	22,31,34	2.51	7 (31%)
1	5HC	F	5	2,1	18,22,23	3.99	9 (50%)	22,31,34	2.61	7 (31%)

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
1	5HC	E	5	2,1	-	2/9/23/24	0/2/2/2
1	5HC	F	5	2,1	-	4/9/23/24	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	5	5HC	C2'-C1'	-7.82	1.31	1.52
1	F	5	5HC	C2'-C1'	-7.77	1.31	1.52
1	E	5	5HC	C2'-C3'	-7.45	1.33	1.52
1	F	5	5HC	C2'-C3'	-7.44	1.34	1.52
1	E	5	5HC	C6-N1	5.89	1.48	1.38
1	E	5	5HC	O4'-C1'	5.88	1.55	1.42
1	F	5	5HC	O4'-C1'	5.81	1.55	1.42
1	F	5	5HC	C6-N1	5.77	1.47	1.38
1	F	5	5HC	C4-N4	5.52	1.48	1.34
1	E	5	5HC	C4-N4	5.46	1.48	1.34
1	E	5	5HC	O4'-C4'	5.16	1.56	1.45
1	F	5	5HC	O4'-C4'	5.11	1.56	1.45
1	E	5	5HC	O3'-C3'	3.69	1.51	1.43
1	F	5	5HC	O3'-C3'	3.67	1.51	1.43
1	F	5	5HC	C4-N3	-3.56	1.28	1.34
1	E	5	5HC	C4-N3	-3.43	1.28	1.34
1	F	5	5HC	C2-N3	2.52	1.41	1.36
1	E	5	5HC	C2-N3	2.48	1.41	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	5	5HC	C3'-C2'-C1'	6.01	117.31	102.60
1	E	5	5HC	C3'-C2'-C1'	5.53	116.13	102.60
1	F	5	5HC	N1-C2-N3	5.37	128.12	118.80
1	E	5	5HC	N1-C2-N3	5.15	127.73	118.80
1	F	5	5HC	C6-N1-C2	-4.96	114.35	120.95
1	E	5	5HC	C6-N1-C2	-4.57	114.86	120.95
1	F	5	5HC	O2-C2-N3	-4.31	115.54	122.33
1	E	5	5HC	O2-C2-N3	-4.12	115.84	122.33
1	F	5	5HC	C4'-O4'-C1'	-3.91	100.21	109.51
1	E	5	5HC	C4'-O4'-C1'	-3.88	100.29	109.51
1	E	5	5HC	C5-C6-N1	-2.76	119.23	122.94
1	F	5	5HC	C5-C6-N1	-2.57	119.48	122.94
1	F	5	5HC	C1'-N1-C2	2.53	122.17	117.83
1	E	5	5HC	C1'-N1-C2	2.08	121.40	117.83

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	F	5	5HC	C4-C5-C5M-O5
1	F	5	5HC	C6-C5-C5M-O5
1	F	5	5HC	O4'-C4'-C5'-O5'
1	E	5	5HC	C6-C5-C5M-O5
1	F	5	5HC	C3'-C4'-C5'-O5'
1	E	5	5HC	C4-C5-C5M-O5

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](#)

1 ligand is 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	EDO	C	401	-	3,3,3	0.45	0	2,2,2	0.39	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	EDO	C	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [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	E	17/18 (94%)	-0.65	0 100 100	73, 91, 153, 163	0
1	F	17/18 (94%)	-0.41	0 100 100	85, 114, 162, 169	0
2	G	14/14 (100%)	-0.58	0 100 100	82, 97, 142, 144	0
2	H	14/14 (100%)	-0.46	0 100 100	89, 109, 140, 152	0
3	A	314/321 (97%)	-0.30	0 100 100	41, 104, 155, 174	0
3	B	313/321 (97%)	-0.44	1 (0%) 90 87	37, 83, 128, 150	0
3	C	314/321 (97%)	-0.35	0 100 100	47, 93, 145, 177	0
3	D	313/321 (97%)	-0.29	1 (0%) 90 87	53, 104, 146, 164	0
All	All	1316/1348 (97%)	-0.36	2 (0%) 91 89	37, 96, 146, 177	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	5	ALA	2.2
3	D	136	LEU	2.1

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	5HC	E	5	21/22	0.84	0.11	102,117,135,145	0
1	5HC	F	5	21/22	0.89	0.09	110,128,141,154	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	EDO	C	401	4/4	0.84	0.14	86,88,89,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.