



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 04:43 pm GMT

PDB ID : 2C5Q
Title : Crystal structure of yeast YER010Cp
Authors : Leulliot, N.; Quevillon-Cheruel, S.; Graille, M.; Schiltz, M.; Blondeau, K.;
Janin, J.; van Tilbeurgh, H.
Deposited on : 2005-10-31
Resolution : 1.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

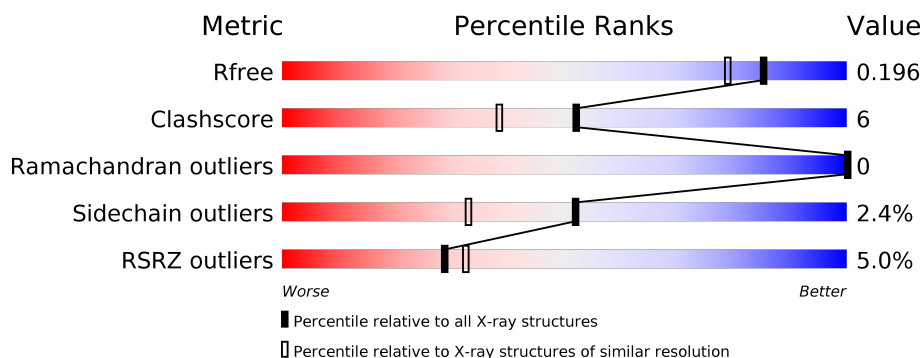
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	111664	3793 (1.70-1.70)
Clashscore	122126	4167 (1.70-1.70)
Ramachandran outliers	120053	4100 (1.70-1.70)
Sidechain outliers	120020	4100 (1.70-1.70)
RSRZ outliers	108989	3718 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>••</div> </div> </div>
1	B	240	<div> <div>7%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>••</div> </div> </div>
1	C	240	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>••</div> </div> </div>
1	D	240	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div>••</div> </div> </div>
1	E	240	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>•</div> </div> </div>
1	F	240	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>••</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	1234	-	-	X	-

2 Entry composition [i](#)

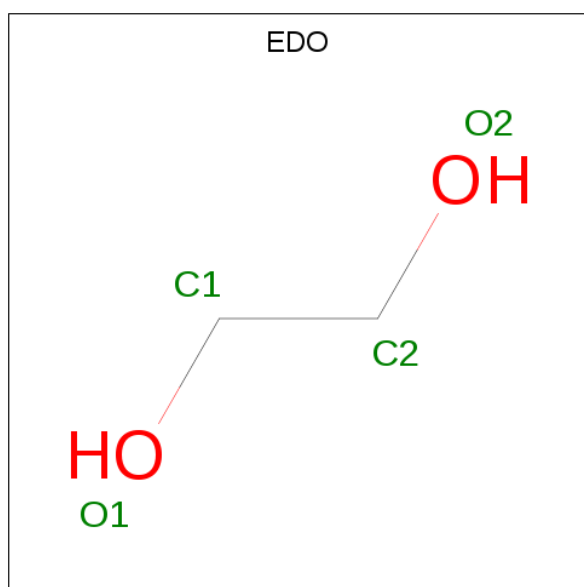
There are 3 unique types of molecules in this entry. The entry contains 12424 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RRAA-LIKE PROTEIN YER010C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	1
			1788	1135	305	342	6			
1	B	232	Total	C	N	O	S	0	0	1
			1776	1126	304	340	6			
1	C	233	Total	C	N	O	S	0	0	1
			1788	1135	305	342	6			
1	D	233	Total	C	N	O	S	0	0	1
			1788	1135	305	342	6			
1	E	234	Total	C	N	O	S	0	0	1
			1796	1141	306	343	6			
1	F	231	Total	C	N	O	S	0	0	1
			1767	1120	302	339	6			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	298	Total O 298 298	0	0
3	B	253	Total O 253 253	0	0
3	C	291	Total O 291 291	0	0
3	D	308	Total O 308 308	0	0
3	E	245	Total O 245 245	0	0
3	F	274	Total O 274 274	0	0

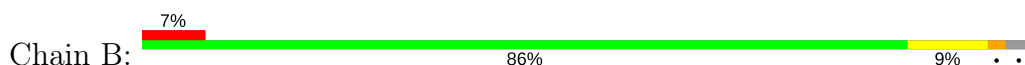
3 Residue-property plots [i](#)

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

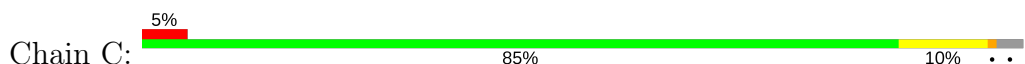
- Molecule 1: RRAA-LIKE PROTEIN YER010C



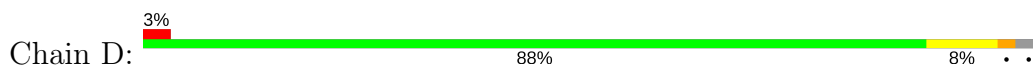
- Molecule 1: RRAA-LIKE PROTEIN YER010C



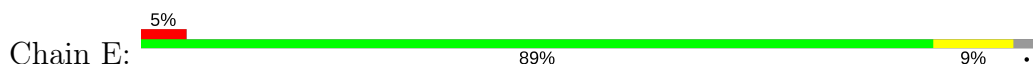
- Molecule 1: RRAA-LIKE PROTEIN YER010C



- Molecule 1: RRAA-LIKE PROTEIN YER010C

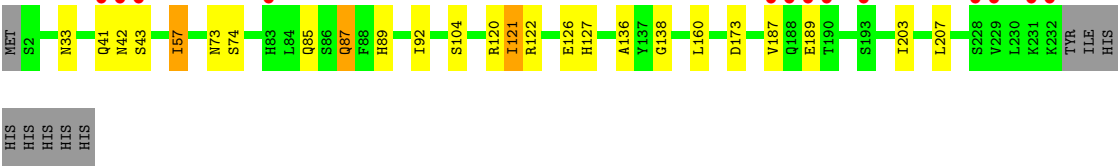
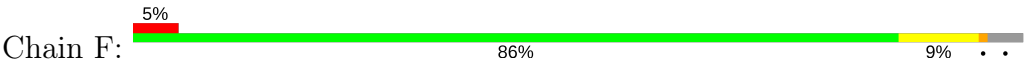


- Molecule 1: RRAA-LIKE PROTEIN YER010C





● Molecule 1: RRAA-LIKE PROTEIN YER010C



HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.19Å 255.07Å 48.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 1.70 19.93 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-1.70) 99.0 (19.93-1.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.155 , 0.183 0.169 , 0.196	Depositor DCC
R_{free} test set	8713 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.8	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12424	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: CME, 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	A	0.72	0/1813	0.77	0/2470
1	B	0.68	0/1800	0.79	1/2452 (0.0%)
1	C	0.69	0/1813	0.77	0/2470
1	D	0.75	1/1813 (0.1%)	0.79	1/2470 (0.0%)
1	E	0.68	0/1821	0.75	0/2481
1	F	0.71	0/1791	0.74	0/2441
All	All	0.71	1/10851 (0.0%)	0.77	2/14784 (0.0%)

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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	189	GLU	CB-CG	-5.20	1.42	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	D	122	ARG	NE-CZ-NH1	5.27	122.94	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	74	SER	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	1788	0	1806	19	0
1	B	1776	0	1797	23	0
1	C	1788	0	1806	27	0
1	D	1788	0	1806	21	0
1	E	1796	0	1817	23	0
1	F	1767	0	1784	28	0
2	A	4	0	6	0	0
2	B	8	0	12	5	0
2	C	4	0	6	0	0
2	D	16	0	24	0	0
2	F	20	0	30	1	0
3	A	298	0	0	1	0
3	B	253	0	0	7	0
3	C	291	0	0	5	0
3	D	308	0	0	7	0
3	E	245	0	0	0	0
3	F	274	0	0	5	0
All	All	12424	0	10894	129	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 6.

All (129) 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:D:192:ILE:HG12	3:D:2244:HOH:O	1.52	1.08
1:D:65:ASN:HD22	1:E:220:LYS:HE3	1.24	0.99
1:A:191:ASP:OD1	1:A:194:LYS:NZ	1.98	0.97
1:C:234:ILE:N	3:C:2289:HOH:O	2.05	0.89
1:F:43:SER:O	3:F:2068:HOH:O	1.90	0.89
1:F:87:GLN:HE21	1:F:87:GLN:H	1.17	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:GLN:HE21	1:C:87:GLN:H	1.23	0.84
1:D:65:ASN:ND2	1:E:220:LYS:HE3	1.91	0.84
1:B:120:ARG:HH22	1:C:33:ASN:HD21	1.25	0.83
1:A:195:LEU:CD1	1:A:199:ILE:HD11	2.10	0.82
1:E:120:ARG:HH22	1:F:33:ASN:HD21	1.26	0.80
1:F:42:ASN:HB2	3:F:2070:HOH:O	1.81	0.79
1:F:203:ILE:O	1:F:207:LEU:HD23	1.83	0.77
2:B:1234:EDO:C2	1:C:180:ASN:HD21	2.00	0.75
1:B:41:GLN:N	3:B:2053:HOH:O	2.21	0.74
1:A:120:ARG:HH22	1:B:33:ASN:HD21	1.33	0.73
1:A:104:SER:OG	1:A:127:HIS:HD2	1.73	0.71
1:D:3:ASP:OD2	3:D:2008:HOH:O	2.10	0.70
1:B:126:GLU:OE1	3:B:2148:HOH:O	2.10	0.70
1:C:42:ASN:HD22	1:C:42:ASN:N	1.90	0.69
1:D:104:SER:OG	1:D:127:HIS:HD2	1.73	0.69
1:D:120:ARG:HH22	1:E:33:ASN:HD21	1.39	0.69
1:D:65:ASN:HD22	1:E:220:LYS:CE	2.02	0.69
1:A:195:LEU:CD1	1:A:199:ILE:CD1	2.72	0.67
1:B:85:GLN:NE2	1:B:160:LEU:H	1.92	0.67
1:D:33:ASN:HD21	1:F:120:ARG:HH22	1.41	0.67
1:B:104:SER:OG	1:B:127:HIS:HD2	1.78	0.66
1:B:186:PRO:O	1:B:190:THR:HG23	1.96	0.65
1:F:87:GLN:H	1:F:87:GLN:NE2	1.93	0.65
1:B:85:GLN:HE22	1:B:160:LEU:H	1.44	0.64
1:A:195:LEU:HD12	1:A:199:ILE:CD1	2.28	0.63
1:E:41:GLN:OE1	1:E:131:ASN:HB3	1.98	0.63
1:E:57:ILE:HD12	1:E:58:ASP:N	2.15	0.62
1:E:85:GLN:HE22	1:E:160:LEU:H	1.48	0.61
1:D:57:ILE:HD13	1:D:57:ILE:H	1.65	0.61
1:A:57:ILE:HD11	3:A:2193:HOH:O	2.01	0.60
1:E:34:LEU:HB2	1:E:182:ILE:HD13	1.83	0.60
1:A:195:LEU:HD11	1:A:199:ILE:HD11	1.83	0.60
1:E:104:SER:OG	1:E:127:HIS:HD2	1.84	0.60
1:F:122:ARG:O	1:F:127:HIS:HE1	1.85	0.59
1:C:122:ARG:O	1:C:127:HIS:HE1	1.84	0.59
1:E:85:GLN:NE2	1:E:160:LEU:H	2.01	0.59
2:B:1234:EDO:H21	1:C:180:ASN:HD21	1.67	0.58
1:A:57:ILE:HD13	1:A:57:ILE:H	1.69	0.58
1:D:85:GLN:NE2	1:D:160:LEU:H	2.00	0.58
1:E:182:ILE:N	1:E:182:ILE:HD12	2.19	0.58
1:D:85:GLN:HE22	1:D:160:LEU:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ARG:HD2	3:B:2227:HOH:O	2.03	0.57
1:D:145:LYS:C	1:D:145:LYS:HD2	2.25	0.57
1:D:104:SER:OG	1:D:127:HIS:CD2	2.57	0.56
1:F:104:SER:OG	1:F:127:HIS:HD2	1.87	0.56
1:D:45:ILE:H	1:D:45:ILE:HD13	1.70	0.56
1:A:195:LEU:HD12	1:A:199:ILE:HD11	1.84	0.56
1:C:104:SER:OG	1:C:127:HIS:HD2	1.89	0.56
1:E:34:LEU:CD1	1:E:182:ILE:HD13	2.36	0.56
1:B:122:ARG:O	1:B:127:HIS:HE1	1.90	0.55
2:B:1234:EDO:H22	1:C:180:ASN:HD21	1.72	0.54
1:A:122:ARG:O	1:A:127:HIS:HE1	1.91	0.54
1:C:85:GLN:NE2	1:C:160:LEU:H	2.05	0.54
1:F:121:ILE:HD13	1:F:138:GLY:O	2.07	0.54
1:E:122:ARG:O	1:E:127:HIS:HE1	1.91	0.54
1:C:42:ASN:ND2	1:C:42:ASN:N	2.56	0.53
1:A:85:GLN:NE2	1:A:160:LEU:H	2.07	0.53
1:F:203:ILE:O	1:F:207:LEU:CD2	2.54	0.53
1:A:104:SER:OG	1:A:127:HIS:CD2	2.58	0.53
1:A:65:ASN:ND2	1:B:220:LYS:HB2	2.24	0.52
1:E:174:TYR:HE2	1:E:192:ILE:HD13	1.74	0.52
1:D:122:ARG:O	1:D:127:HIS:HE1	1.93	0.52
1:A:85:GLN:HE22	1:A:160:LEU:H	1.56	0.52
1:F:121:ILE:H	1:F:121:ILE:HD13	1.74	0.52
1:D:234:ILE:N	3:D:2302:HOH:O	2.44	0.51
1:C:85:GLN:HE22	1:C:160:LEU:H	1.57	0.51
1:B:104:SER:OG	1:B:127:HIS:CD2	2.63	0.51
1:B:201:LYS:HB2	1:B:201:LYS:HZ3	1.76	0.51
1:C:84:LEU:HD12	3:C:2083:HOH:O	2.10	0.51
1:E:181:GLY:C	1:E:182:ILE:HD12	2.32	0.51
1:C:87:GLN:H	1:C:87:GLN:NE2	2.00	0.50
1:F:73:ASN:ND2	3:F:2148:HOH:O	2.45	0.50
1:C:57:ILE:HD12	1:C:58:ASP:N	2.25	0.50
1:B:45:ILE:HD13	1:B:45:ILE:H	1.77	0.50
1:B:126:GLU:HG3	3:B:2149:HOH:O	2.11	0.50
1:D:89:HIS:HB2	1:F:89:HIS:CD2	2.47	0.49
1:C:174:TYR:HE1	1:C:192:ILE:HD13	1.78	0.49
1:F:85:GLN:HE22	1:F:160:LEU:H	1.61	0.49
1:A:89:HIS:HB2	1:C:89:HIS:CD2	2.47	0.49
1:F:85:GLN:NE2	1:F:160:LEU:H	2.11	0.49
1:C:232:LYS:HE3	1:C:232:LYS:H	1.78	0.48
1:F:57:ILE:HD13	1:F:57:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:191:ASP:OD2	3:D:2246:HOH:O	2.20	0.47
1:F:126:GLU:H	2:F:1232:EDO:H22	1.78	0.47
1:B:87:GLN:NE2	3:B:2111:HOH:O	2.42	0.47
3:D:2177:HOH:O	1:E:43:SER:HB2	2.14	0.47
1:E:89:HIS:HB3	1:F:89:HIS:HB3	1.97	0.47
1:F:57:ILE:HD13	1:F:57:ILE:H	1.79	0.47
1:C:186:PRO:O	1:C:190:THR:OG1	2.26	0.47
1:B:201:LYS:NZ	1:B:201:LYS:HB2	2.30	0.47
1:B:227:ARG:HG2	1:B:231:LYS:HD3	1.98	0.46
1:E:104:SER:OG	1:E:127:HIS:CD2	2.68	0.46
1:F:104:SER:OG	1:F:127:HIS:CD2	2.68	0.45
1:C:232:LYS:NZ	3:C:2286:HOH:O	2.50	0.45
1:F:87:GLN:HE21	1:F:87:GLN:N	1.99	0.45
1:D:192:ILE:CG1	3:D:2244:HOH:O	2.34	0.45
1:E:41:GLN:OE1	1:E:131:ASN:CB	2.65	0.45
1:B:220:LYS:NZ	3:B:2238:HOH:O	2.50	0.44
1:C:73:ASN:ND2	3:C:2123:HOH:O	2.50	0.44
1:F:173:ASP:HA	1:F:187:VAL:HG13	2.00	0.43
1:A:195:LEU:HD12	1:A:199:ILE:HD12	1.98	0.43
1:B:34:LEU:HD13	1:B:182:ILE:HG13	2.00	0.43
1:C:122:ARG:O	1:C:127:HIS:CE1	2.69	0.43
1:F:207:LEU:HD22	3:F:2239:HOH:O	2.17	0.43
3:D:2026:HOH:O	1:E:220:LYS:HE2	2.19	0.42
1:C:194:LYS:NZ	1:C:194:LYS:HB2	2.34	0.42
1:C:87:GLN:HE21	1:C:87:GLN:N	2.03	0.42
1:F:189:GLU:N	1:F:189:GLU:OE2	2.52	0.42
1:D:145:LYS:HD2	1:D:146:ALA:N	2.35	0.42
2:B:1234:EDO:C1	3:C:2022:HOH:O	2.67	0.42
1:D:34:LEU:HD13	1:D:182:ILE:HG13	2.02	0.42
1:E:89:HIS:CG	1:E:90:PRO:HA	2.54	0.42
1:B:85:GLN:HE22	1:B:160:LEU:N	2.15	0.42
1:F:121:ILE:HD12	1:F:136:ALA:HB3	2.02	0.42
1:A:89:HIS:HB3	1:B:89:HIS:HB3	2.02	0.41
1:C:191:ASP:OD2	1:C:194:LYS:NZ	2.53	0.41
1:C:117:VAL:O	1:C:136:ALA:HA	2.20	0.41
1:F:126:GLU:HG3	3:F:2159:HOH:O	2.20	0.41
3:B:2114:HOH:O	1:C:88:PHE:HD1	2.02	0.41
1:F:42:ASN:HB3	1:F:43:SER:H	1.66	0.41
1:A:47:GLY:HA3	1:A:75:ILE:HG12	2.03	0.40
1:E:34:LEU:HD12	1:E:182:ILE:HD13	2.02	0.40
1:B:123:ASP:HA	2:B:1234:EDO:H22	2.02	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	230/240 (96%)	223 (97%)	7 (3%)	0	100	100
1	B	229/240 (95%)	222 (97%)	7 (3%)	0	100	100
1	C	230/240 (96%)	223 (97%)	7 (3%)	0	100	100
1	D	230/240 (96%)	224 (97%)	6 (3%)	0	100	100
1	E	231/240 (96%)	225 (97%)	6 (3%)	0	100	100
1	F	228/240 (95%)	221 (97%)	7 (3%)	0	100	100
All	All	1378/1440 (96%)	1338 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	201/209 (96%)	197 (98%)	4 (2%)	58	40
1	B	200/209 (96%)	192 (96%)	8 (4%)	34	14
1	C	201/209 (96%)	195 (97%)	6 (3%)	44	24
1	D	201/209 (96%)	196 (98%)	5 (2%)	50	31
1	E	202/209 (97%)	201 (100%)	1 (0%)	90	85
1	F	199/209 (95%)	194 (98%)	5 (2%)	50	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1204/1254 (96%)	1175 (98%)	29 (2%)	52 33

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	92	ILE
1	A	195	LEU
1	A	231	LYS
1	B	45	ILE
1	B	58	ASP
1	B	92	ILE
1	B	188	GLN
1	B	201	LYS
1	B	220	LYS
1	B	231	LYS
1	B	232	LYS
1	C	42	ASN
1	C	43	SER
1	C	87	GLN
1	C	92	ILE
1	C	231	LYS
1	C	232	LYS
1	D	45	ILE
1	D	57	ILE
1	D	92	ILE
1	D	145	LYS
1	D	231	LYS
1	E	92	ILE
1	F	41	GLN
1	F	57	ILE
1	F	87	GLN
1	F	92	ILE
1	F	121	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	8	GLN
1	A	85	GLN

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Mol	Chain	Res	Type
1	A	127	HIS
1	B	5	GLN
1	B	8	GLN
1	B	33	ASN
1	B	41	GLN
1	B	85	GLN
1	B	127	HIS
1	B	221	GLN
1	C	8	GLN
1	C	33	ASN
1	C	42	ASN
1	C	73	ASN
1	C	85	GLN
1	C	87	GLN
1	C	89	HIS
1	C	127	HIS
1	C	180	ASN
1	C	224	ASN
1	D	5	GLN
1	D	33	ASN
1	D	73	ASN
1	D	85	GLN
1	D	127	HIS
1	E	5	GLN
1	E	33	ASN
1	E	42	ASN
1	E	65	ASN
1	E	85	GLN
1	E	127	HIS
1	E	154	ASN
1	E	215	ASN
1	F	8	GLN
1	F	33	ASN
1	F	73	ASN
1	F	85	GLN
1	F	87	GLN
1	F	89	HIS
1	F	127	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	CME	A	170	1	9,9,10	0.79	0	6,9,11	0.89	0
1	CME	B	170	1	9,9,10	0.78	0	6,9,11	0.98	1 (16%)
1	CME	C	170	1	9,9,10	0.69	0	6,9,11	1.38	1 (16%)
1	CME	D	170	1	9,9,10	0.73	0	6,9,11	0.87	0
1	CME	E	170	1	9,9,10	0.70	0	6,9,11	0.69	0
1	CME	F	170	1	9,9,10	0.73	0	6,9,11	1.11	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
1	CME	A	170	1	-	0/5/8/10	0/0/0/0
1	CME	B	170	1	-	0/5/8/10	0/0/0/0
1	CME	C	170	1	-	0/5/8/10	0/0/0/0
1	CME	D	170	1	-	0/5/8/10	0/0/0/0
1	CME	E	170	1	-	0/5/8/10	0/0/0/0
1	CME	F	170	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	CME	CE-SD-SG	2.21	114.11	103.47
1	C	170	CME	CE-SD-SG	2.87	117.30	103.47

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	1234	-	3,3,3	0.49	0	2,2,2	0.84	0
2	EDO	B	1233	-	3,3,3	0.36	0	2,2,2	0.41	0
2	EDO	B	1234	-	3,3,3	0.18	0	2,2,2	0.37	0
2	EDO	C	1234	-	3,3,3	0.42	0	2,2,2	0.08	0
2	EDO	D	1234	-	3,3,3	0.78	0	2,2,2	0.22	0
2	EDO	D	1235	-	3,3,3	0.37	0	2,2,2	0.65	0
2	EDO	D	1236	-	3,3,3	0.40	0	2,2,2	0.56	0
2	EDO	D	1237	-	3,3,3	0.37	0	2,2,2	0.43	0
2	EDO	F	1232	-	3,3,3	0.36	0	2,2,2	0.23	0
2	EDO	F	1233	-	3,3,3	0.38	0	2,2,2	0.70	0
2	EDO	F	1234	-	3,3,3	0.57	0	2,2,2	0.26	0
2	EDO	F	1235	-	3,3,3	0.44	0	2,2,2	0.48	0
2	EDO	F	1236	-	3,3,3	0.51	0	2,2,2	0.05	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	EDO	A	1234	-	-	0/1/1/1	0/0/0/0
2	EDO	B	1233	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	1234	-	-	0/1/1/1	0/0/0/0
2	EDO	C	1234	-	-	0/1/1/1	0/0/0/0
2	EDO	D	1234	-	-	0/1/1/1	0/0/0/0
2	EDO	D	1235	-	-	0/1/1/1	0/0/0/0
2	EDO	D	1236	-	-	0/1/1/1	0/0/0/0
2	EDO	D	1237	-	-	0/1/1/1	0/0/0/0
2	EDO	F	1232	-	-	0/1/1/1	0/0/0/0
2	EDO	F	1233	-	-	0/1/1/1	0/0/0/0
2	EDO	F	1234	-	-	0/1/1/1	0/0/0/0
2	EDO	F	1235	-	-	0/1/1/1	0/0/0/0
2	EDO	F	1236	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1234	EDO	5	0
2	F	1232	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/240 (96%)	-0.03	9 (3%) 39 44	8, 12, 23, 41	0
1	B	231/240 (96%)	0.15	17 (7%) 14 17	9, 14, 31, 41	0
1	C	232/240 (96%)	0.04	12 (5%) 27 30	8, 12, 27, 39	0
1	D	232/240 (96%)	0.02	7 (3%) 50 55	8, 12, 25, 40	0
1	E	233/240 (97%)	0.13	12 (5%) 27 30	8, 14, 29, 38	0
1	F	230/240 (95%)	0.12	13 (5%) 24 26	8, 13, 29, 39	0
All	All	1390/1440 (96%)	0.07	70 (5%) 29 32	8, 13, 29, 41	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	42	ASN	6.9
1	F	43	SER	6.6
1	D	233	TYR	6.3
1	A	234	ILE	6.0
1	E	43	SER	5.7
1	D	43	SER	5.5
1	B	41	GLN	5.4
1	F	188	GLN	5.2
1	A	42	ASN	5.1
1	D	41	GLN	5.1
1	B	42	ASN	5.0
1	A	233	TYR	5.0
1	B	43	SER	4.9
1	F	232	LYS	4.9
1	C	43	SER	4.8
1	E	41	GLN	4.8
1	B	4	LEU	4.8
1	A	43	SER	4.6
1	D	42	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	42	ASN	4.6
1	F	42	ASN	4.6
1	F	231	LYS	4.4
1	A	41	GLN	4.4
1	B	2	SER	4.4
1	A	232	LYS	4.2
1	C	188	GLN	3.9
1	B	227	ARG	3.9
1	D	232	LYS	3.8
1	E	231	LYS	3.8
1	B	5	GLN	3.7
1	F	189	GLU	3.7
1	C	232	LYS	3.7
1	E	188	GLN	3.6
1	B	232	LYS	3.6
1	D	231	LYS	3.4
1	E	234	ILE	3.4
1	C	231	LYS	3.3
1	D	234	ILE	3.3
1	B	9	ARG	3.2
1	B	188	GLN	3.2
1	B	231	LYS	3.0
1	E	2	SER	2.9
1	C	41	GLN	2.9
1	B	189	GLU	2.9
1	F	228	SER	2.8
1	C	233	TYR	2.8
1	C	58	ASP	2.8
1	B	3	ASP	2.7
1	C	5	GLN	2.6
1	F	190	THR	2.6
1	C	189	GLU	2.6
1	F	229	VAL	2.6
1	F	83	HIS	2.5
1	B	24	ASN	2.5
1	B	6	LYS	2.4
1	F	41	GLN	2.4
1	E	189	GLU	2.4
1	C	234	ILE	2.3
1	B	58	ASP	2.3
1	E	192	ILE	2.3
1	E	190	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	9	ARG	2.1
1	A	58	ASP	2.1
1	F	193	SER	2.1
1	A	131	ASN	2.1
1	E	225	ASP	2.1
1	C	57	ILE	2.1
1	B	39	PRO	2.0
1	F	187	VAL	2.0
1	A	231	LYS	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
1	CME	C	170	10/11	0.92	0.14	12,14,38,43	0
1	CME	F	170	10/11	0.93	0.17	12,14,38,41	0
1	CME	E	170	10/11	0.93	0.18	13,16,41,44	0
1	CME	B	170	10/11	0.93	0.15	14,15,40,43	0
1	CME	A	170	10/11	0.94	0.15	10,12,35,37	0
1	CME	D	170	10/11	0.94	0.13	11,13,33,37	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å ²)	Q<0.9
2	EDO	B	1234	4/4	0.83	0.19	23,26,26,28	0
2	EDO	D	1234	4/4	0.88	0.14	22,24,25,25	0
2	EDO	F	1235	4/4	0.90	0.10	32,33,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	F	1232	4/4	0.90	0.18	20,21,24,31	0
2	EDO	A	1234	4/4	0.90	0.14	15,17,18,18	0
2	EDO	F	1234	4/4	0.93	0.09	22,23,24,25	0
2	EDO	B	1233	4/4	0.94	0.08	20,25,26,26	0
2	EDO	D	1237	4/4	0.95	0.10	19,21,24,27	0
2	EDO	F	1233	4/4	0.95	0.11	19,23,23,24	0
2	EDO	D	1236	4/4	0.95	0.09	22,26,27,30	0
2	EDO	D	1235	4/4	0.96	0.08	16,19,19,20	0
2	EDO	C	1234	4/4	0.96	0.10	23,25,28,28	0
2	EDO	F	1236	4/4	0.97	0.08	20,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.