



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:13 AM UTC

PDB ID : 6FKX / pdb_00006fkx
Title : Crystal structure of an acetyl xylan esterase from a desert metagenome
Authors : Adesioye, F.A.; Makhalanyaane, T.P.; Vikram, S.; Sewell, B.T.; Schubert, W.; Cowan, D.A.
Deposited on : 2018-01-24
Resolution : 2.03 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

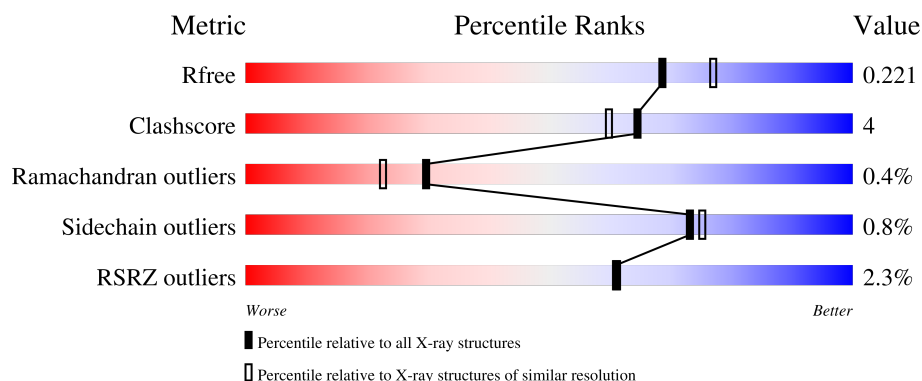
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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.



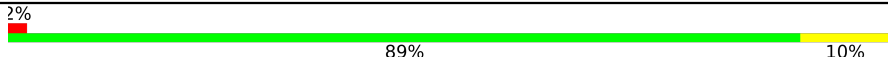
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	324	 3% 94% 6%
2	B	322	 3% 89% 10%
2	D	322	 2% 93% 7%
2	E	322	 2% 88% 12%
2	F	322	 2% 90% 9% ..

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Mol	Chain	Length	Quality of chain
3	C	319	 A horizontal bar chart showing the quality of chain 3. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '89%', and a small yellow segment at the end labeled '10%'.

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
5	MES	F	402	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 17799 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 Acetyl xylan esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	4	1
			2566	1639	446	472	9			

- Molecule 2 is a protein called Acetyl xylan esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	11	0
			2591	1659	444	479	9			
2	D	322	Total	C	N	O	S	0	6	0
			2560	1637	441	473	9			
2	E	322	Total	C	N	O	S	0	5	0
			2554	1633	444	468	9			
2	F	322	Total	C	N	O	S	0	12	0
			2604	1667	455	473	9			

- Molecule 3 is a protein called Acetyl xylan esterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	319	Total	C	N	O	S	0	8	0
			2548	1629	443	467	9			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

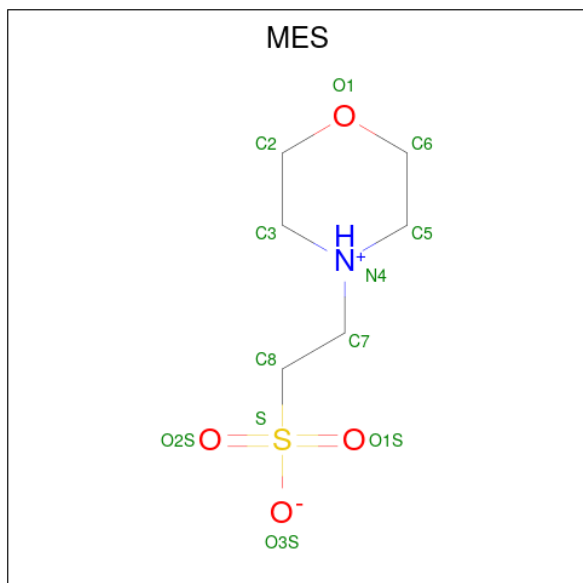
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			8	3	1	3	1		
5	B	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
5	B	1	Total	C	O	S		0	0
			5	1	3	1			
5	D	1	Total	C	N	O	S	0	0
			8	3	1	3	1		
5	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	D	1	Total	C	N	O	S	0	0
			11	5	1	4	1		
5	C	1	Total	C	O	S		0	0
			6	2	3	1			
5	C	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
5	C	1	Total	C	O	S		0	0
			6	2	3	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
5	E	1	Total	C	O	S		0	0
			6	2	3	1			
5	F	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
5	F	1	Total	C	N	O	S	0	0
			8	3	1	3	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

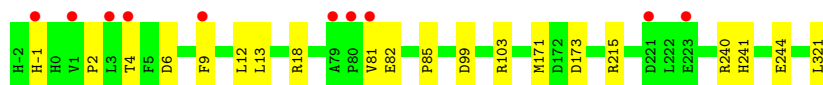
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	350	Total	O	0	0
			350	350		
8	B	366	Total	O	0	0
			366	366		
8	D	379	Total	O	0	0
			379	379		
8	C	377	Total	O	0	0
			377	377		
8	E	367	Total	O	0	0
			367	367		
8	F	425	Total	O	0	0
			425	425		

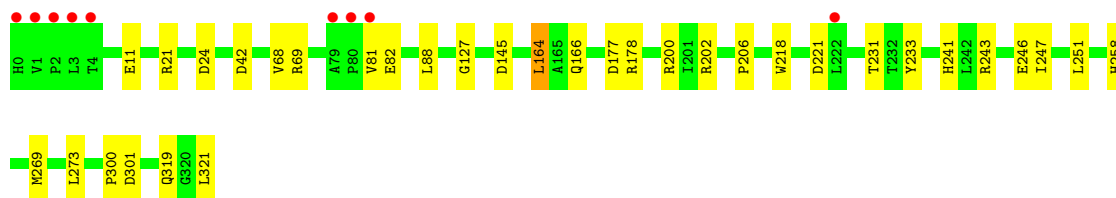
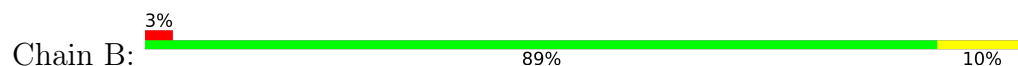
3 Residue-property plots [i](#)

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: Acetyl xylan esterase



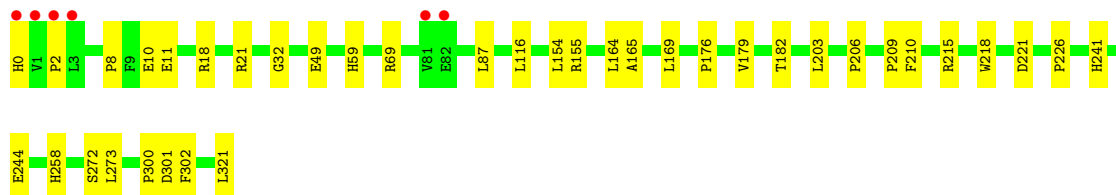
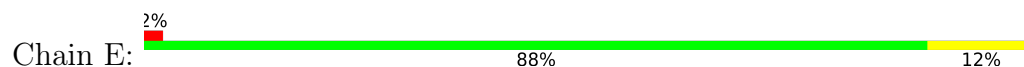
- Molecule 2: Acetyl xylan esterase



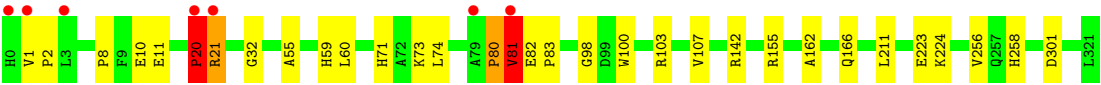
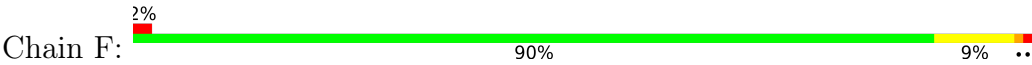
- Molecule 2: Acetyl xylan esterase



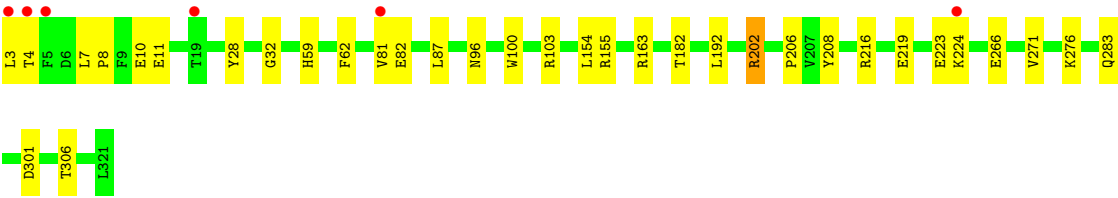
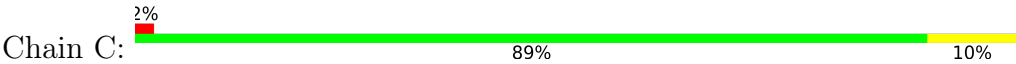
- Molecule 2: Acetyl xylan esterase



- Molecule 2: Acetyl xylan esterase



● Molecule 3: Acetyl xylan esterase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.68Å 116.82Å 159.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.23 – 2.03 89.23 – 2.03	Depositor EDS
% Data completeness (in resolution range)	100.0 (89.23-2.03) 100.0 (89.23-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.03Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.169 , 0.220 0.170 , 0.221	Depositor DCC
R_{free} test set	6726 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17799	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: NA, FMT, SO4, MES

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	0.17	0/2649	0.41	0/3616
2	B	0.17	0/2697	0.40	0/3683
2	D	0.17	0/2651	0.39	0/3621
2	E	0.18	0/2642	0.39	0/3609
2	F	0.22	0/2713	0.50	3/3700 (0.1%)
3	C	0.21	0/2643	0.48	2/3605 (0.1%)
All	All	0.19	0/15995	0.43	5/21834 (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
3	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	224	LYS	CB-CA-C	6.46	123.27	110.42
2	F	81	VAL	CA-CB-CG2	6.07	120.72	110.40
3	C	224	LYS	N-CA-CB	-5.89	100.54	110.49
2	F	20	PRO	CA-C-N	5.25	134.62	121.80
2	F	20	PRO	C-N-CA	5.25	134.62	121.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	223	GLU	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	2566	0	2492	14	0
2	B	2591	0	2536	25	0
2	D	2560	0	2494	19	0
2	E	2554	0	2496	25	0
2	F	2604	0	2572	20	0
3	C	2548	0	2496	21	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	8	0	4	0	0
5	B	12	0	4	0	0
5	C	19	0	8	3	0
5	D	31	0	24	5	0
5	E	13	0	6	4	0
5	F	15	0	8	3	0
6	A	5	0	0	0	0
7	B	3	0	1	0	0
8	A	350	0	0	4	0
8	B	366	0	0	7	0
8	C	377	0	0	5	0
8	D	379	0	0	3	0
8	E	367	0	0	0	0
8	F	425	0	0	0	0
All	All	17799	0	15141	120	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 4.

All (120) 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)
2:F:223[A]:GLU:HG2	2:F:224:LYS:HG3	1.48	0.94
1:A:99:ASP:O	1:A:103:ARG:NH2	2.12	0.83
1:A:4:THR:HG22	1:A:6:ASP:H	1.48	0.77
2:E:49:GLU:H	5:E:402:MES:H81	1.52	0.74
1:A:81:VAL:HG23	1:A:82:GLU:HG3	1.72	0.72
3:C:59:HIS:HE1	5:C:403:MES:H81	1.56	0.68
2:F:73[A]:LYS:NZ	2:F:98:GLY:O	2.24	0.67
2:B:206:PRO:HG2	2:B:269:MET:HG3	1.77	0.67
3:C:59:HIS:CE1	5:C:403:MES:H81	2.32	0.64
2:B:202:ARG:NH1	2:B:321:LEU:O	2.31	0.64
2:E:241:HIS:NE2	2:F:301:ASP:OD2	2.23	0.64
1:A:2:PRO:HG2	3:C:219:GLU:HB3	1.83	0.61
3:C:11:GLU:OE1	8:C:501:HOH:O	2.16	0.61
3:C:3:LEU:O	3:C:4:THR:HG23	2.01	0.60
2:D:81:VAL:HG13	2:D:82:GLU:H	1.68	0.58
2:D:59:HIS:HE1	5:D:402:MES:H72	1.69	0.57
2:D:287:TYR:HA	2:D:290:LEU:HD22	1.85	0.57
2:F:21:ARG:HB2	2:F:258:HIS:CE1	2.40	0.57
2:F:8:PRO:HG2	2:F:11:GLU:HG3	1.88	0.56
3:C:81:VAL:HG23	3:C:82:GLU:H	1.71	0.56
2:F:73[B]:LYS:NZ	2:F:98:GLY:O	2.30	0.56
1:A:85:PRO:HB3	1:A:321:LEU:HD13	1.87	0.55
2:B:24:ASP:OD2	8:B:502:HOH:O	2.18	0.54
2:E:215:ARG:NH2	2:E:244:GLU:OE1	2.40	0.54
2:D:208:TYR:HA	2:D:283:GLN:NE2	2.24	0.53
1:A:215:ARG:NH1	1:A:244:GLU:OE1	2.38	0.52
1:A:18[B]:ARG:NH1	8:A:510:HOH:O	2.41	0.52
2:B:221[A]:ASP:OD1	8:B:503:HOH:O	2.19	0.52
2:F:100:TRP:HE1	5:F:402:MES:H81	1.73	0.52
1:A:173:ASP:OD2	8:A:501:HOH:O	2.19	0.52
2:E:206:PRO:HB2	2:E:209:PRO:HG3	1.93	0.51
1:A:240:ARG:NH1	8:A:513:HOH:O	2.43	0.51
2:D:215:ARG:NE	8:D:508:HOH:O	2.42	0.51
2:F:60:LEU:HD12	2:F:74:LEU:HD22	1.93	0.51
2:B:241:HIS:NE2	3:C:301:ASP:OD2	2.31	0.51
3:C:8:PRO:HB2	3:C:10:GLU:OE2	2.12	0.50
2:B:68[A]:VAL:HG13	2:B:127:GLY:HA3	1.94	0.50
2:F:211:LEU:O	2:F:256[B]:VAL:HG13	2.12	0.50
2:F:59:HIS:HD2	2:F:71:HIS:NE2	2.09	0.50
2:B:202:ARG:NH2	8:B:527:HOH:O	2.45	0.49
2:E:18[A]:ARG:NH1	2:F:2:PRO:HD3	2.26	0.49
2:F:59:HIS:NE2	5:F:402:MES:H71	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246[B]:GLU:HG3	2:B:247:ILE:N	2.27	0.49
2:E:165:ALA:O	2:E:169:LEU:HD23	2.12	0.49
2:D:273:LEU:HB2	2:D:300:PRO:HA	1.95	0.48
2:E:21:ARG:HB2	2:E:258:HIS:CE1	2.48	0.48
3:C:202[A]:ARG:NH2	8:C:520:HOH:O	2.45	0.48
2:E:49:GLU:HB3	5:E:402:MES:H72	1.96	0.48
2:B:177:ASP:OD2	2:B:200[A]:ARG:NH2	2.39	0.48
2:D:59:HIS:CE1	5:D:402:MES:H72	2.49	0.48
1:A:241:HIS:NE2	2:B:301:ASP:OD2	2.26	0.48
2:B:177:ASP:O	2:B:202:ARG:HD3	2.14	0.47
2:D:87:LEU:HD11	2:D:182:THR:HG22	1.96	0.47
3:C:7:LEU:HD13	3:C:216:ARG:NH2	2.29	0.47
2:D:100:TRP:HE1	5:D:402:MES:H81	1.79	0.47
2:E:273:LEU:HB2	2:E:300:PRO:HA	1.97	0.47
3:C:96:ASN:ND2	8:C:523:HOH:O	2.46	0.47
1:A:9:PHE:HA	1:A:12:LEU:HD12	1.95	0.47
2:D:218:TRP:CZ2	2:D:241:HIS:HE1	2.33	0.47
2:D:289:LYS:NZ	8:D:507:HOH:O	2.41	0.47
2:B:81:VAL:HG23	2:B:82[A]:GLU:H	1.80	0.46
2:B:145:ASP:OD2	2:B:233:TYR:OH	2.30	0.46
2:D:99:ASP:O	2:D:103[A]:ARG:NH1	2.48	0.46
2:F:32:GLY:HA2	2:F:155[A]:ARG:NH2	2.30	0.46
2:E:116:LEU:HB2	2:E:164:LEU:HD22	1.96	0.46
2:B:178[B]:ARG:HD2	2:B:321:LEU:O	2.15	0.46
5:D:404:MES:H81	5:D:404:MES:H52	1.65	0.46
1:A:171:MET:HB3	1:A:173:ASP:OD1	2.16	0.46
3:C:81:VAL:HG23	3:C:82:GLU:HG2	1.98	0.46
2:B:218:TRP:CZ2	2:B:241:HIS:HE1	2.34	0.46
3:C:28:TYR:OH	3:C:155:ARG:HD2	2.16	0.46
2:E:59:HIS:CE1	5:E:402:MES:H82	2.51	0.45
3:C:192:LEU:HD21	3:C:206:PRO:HG3	1.98	0.45
3:C:208:TYR:HA	3:C:283:GLN:OE1	2.16	0.45
2:E:10:GLU:HG3	2:E:11:GLU:N	2.31	0.45
2:B:81:VAL:HG23	2:B:82[B]:GLU:H	1.80	0.45
2:B:166:GLN:NE2	8:B:517:HOH:O	2.39	0.45
2:F:55:ALA:HB2	2:F:107:VAL:HG11	1.99	0.45
2:E:169:LEU:HD22	2:E:179:VAL:HG21	1.98	0.44
2:E:59:HIS:NE2	5:E:402:MES:H82	2.33	0.44
2:F:82:GLU:HG3	2:F:83:PRO:HD2	2.00	0.44
2:E:32:GLY:HA2	2:E:155:ARG:NH2	2.33	0.44
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:100:TRP:HE1	5:C:403:MES:H82	1.83	0.44
2:D:136:MET:O	5:D:404:MES:H61	2.18	0.43
3:C:266:GLU:OE1	8:C:502:HOH:O	2.21	0.43
2:B:243:ARG:HB3	2:B:246[B]:GLU:HG2	2.00	0.43
2:F:20:PRO:O	2:F:21:ARG:HB3	2.18	0.43
2:B:42:ASP:HB3	2:B:69:ARG:HH12	1.83	0.43
3:C:62:PHE:CD1	3:C:163:ARG:HG2	2.54	0.43
3:C:276[B]:LYS:NZ	8:C:533:HOH:O	2.52	0.43
2:E:8:PRO:HG2	2:E:11:GLU:HG3	2.01	0.43
1:A:215:ARG:NE	8:A:522:HOH:O	2.51	0.43
2:E:218:TRP:CZ2	2:E:241:HIS:HE1	2.37	0.42
2:F:142:ARG:HD2	5:F:403:MES:N4	2.34	0.42
3:C:87:LEU:HD11	3:C:182:THR:HG22	2.02	0.42
2:D:31:ARG:HD3	8:D:585:HOH:O	2.20	0.42
2:E:210:PHE:CZ	2:E:226:PRO:HB2	2.54	0.42
2:B:21:ARG:HB2	2:B:258:HIS:CE1	2.55	0.42
2:D:116:LEU:HB2	2:D:164:LEU:HD22	2.01	0.42
3:C:32:GLY:HA2	3:C:155:ARG:NH2	2.35	0.42
2:B:88:LEU:HD22	2:B:164:LEU:HD13	2.02	0.41
2:D:81:VAL:HG13	2:D:82:GLU:N	2.33	0.41
2:D:241:HIS:NE2	2:E:301:ASP:OD2	2.33	0.41
2:E:169:LEU:HD13	2:E:176:PRO:HA	2.02	0.41
2:E:87:LEU:HD11	2:E:182:THR:HG22	2.01	0.41
2:F:80:PRO:O	2:F:81:VAL:HG22	2.20	0.41
2:B:319:GLN:NE2	8:B:518:HOH:O	2.39	0.41
2:E:69:ARG:HA	2:E:69:ARG:HD2	1.92	0.41
2:B:273:LEU:HB2	2:B:300:PRO:HA	2.03	0.41
2:D:89:GLN:OE1	2:D:103[B]:ARG:HD3	2.21	0.41
2:E:272:SER:HB2	2:E:302:PHE:O	2.21	0.41
2:E:0:HIS:ND1	2:E:2:PRO:HD3	2.36	0.40
2:E:203:LEU:HD12	2:E:321:LEU:HD13	2.03	0.40
2:F:162:ALA:O	2:F:166:GLN:HG3	2.21	0.40
2:F:10[A]:GLU:CD	2:F:10[A]:GLU:H	2.29	0.40
1:A:9:PHE:CZ	1:A:13:LEU:HD11	2.57	0.40
2:B:231:THR:OG1	8:B:504:HOH:O	2.22	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	326/324 (101%)	315 (97%)	10 (3%)	1 (0%)	36	31
2	B	331/322 (103%)	320 (97%)	11 (3%)	0	100	100
2	D	326/322 (101%)	318 (98%)	7 (2%)	1 (0%)	36	31
2	E	325/322 (101%)	313 (96%)	11 (3%)	1 (0%)	36	31
2	F	332/322 (103%)	320 (96%)	7 (2%)	5 (2%)	8	3
3	C	325/319 (102%)	314 (97%)	11 (3%)	0	100	100
All	All	1965/1931 (102%)	1900 (97%)	57 (3%)	8 (0%)	30	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	HIS
2	F	20	PRO
2	F	21	ARG
2	F	81	VAL
2	F	1	VAL
2	D	81	VAL
2	E	221	ASP
2	F	80	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/263 (101%)	266 (100%)	0	100	100
2	B	272/261 (104%)	268 (98%)	4 (2%)	57	59
2	D	267/261 (102%)	264 (99%)	3 (1%)	65	68
2	E	266/261 (102%)	265 (100%)	1 (0%)	84	84
2	F	273/261 (105%)	272 (100%)	1 (0%)	84	84
3	C	265/258 (103%)	257 (97%)	8 (3%)	36	32
All	All	1609/1565 (103%)	1592 (99%)	17 (1%)	73	68

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	11[A]	GLU
2	B	11[B]	GLU
2	B	164	LEU
2	B	251	LEU
2	D	103[A]	ARG
2	D	103[B]	ARG
2	D	290	LEU
3	C	103	ARG
3	C	154[A]	LEU
3	C	154[B]	LEU
3	C	202[A]	ARG
3	C	202[B]	ARG
3	C	271	VAL
3	C	306[A]	THR
3	C	306[B]	THR
2	E	154	LEU
2	F	103	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	319	GLN
2	B	319	GLN
2	D	258	HIS
2	D	283	GLN

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Mol	Chain	Res	Type
2	E	228	ASN
2	F	59	HIS
2	F	228	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 for Mogul analysis.

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	$\# Z > 2$
5	MES	E	403	-	4,5,12	0.92	0	7,7,16	1.39	1 (14%)
5	MES	C	403	-	6,6,12	3.24	1 (16%)	7,8,16	1.81	2 (28%)
5	MES	F	403	-	7,7,12	2.98	1 (14%)	8,9,16	1.83	3 (37%)
5	MES	A	402	-	7,7,12	3.01	1 (14%)	8,9,16	1.83	3 (37%)
5	MES	B	403	-	4,4,12	0.98	0	6,6,16	0.65	0
5	MES	C	404	-	4,5,12	0.94	0	7,7,16	1.43	1 (14%)
5	MES	D	403	-	12,12,12	2.22	1 (8%)	15,16,16	2.16	6 (40%)
5	MES	E	402	-	6,6,12	3.35	1 (16%)	7,8,16	1.71	2 (28%)
5	MES	F	402	-	6,6,12	3.22	1 (16%)	7,8,16	1.98	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	A	403	-	4,4,4	0.24	0	6,6,6	0.11	0
5	MES	B	402	-	6,6,12	3.24	1 (16%)	7,8,16	1.71	1 (14%)
5	MES	D	404	-	10,10,12	2.57	1 (10%)	11,12,16	1.46	1 (9%)
5	MES	D	402	-	7,7,12	3.05	1 (14%)	8,9,16	1.76	2 (25%)
7	FMT	B	404	-	2,2,2	0.73	0	1,1,1	0.23	0
5	MES	C	402	-	4,5,12	0.94	0	7,7,16	1.45	1 (14%)

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
5	MES	E	403	-	-	0/3/3/14	-
5	MES	C	403	-	-	3/4/4/14	-
5	MES	F	403	-	-	2/5/5/14	-
5	MES	A	402	-	-	0/5/5/14	-
5	MES	C	404	-	-	3/3/3/14	-
5	MES	E	402	-	-	3/4/4/14	-
5	MES	D	403	-	-	2/6/14/14	0/1/1/1
5	MES	F	402	-	-	4/4/4/14	-
5	MES	D	404	-	-	6/8/8/14	-
5	MES	B	402	-	-	4/4/4/14	-
5	MES	D	402	-	-	4/5/5/14	-
5	MES	C	402	-	-	3/3/3/14	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	402	MES	C8-S	-8.00	1.66	1.77
5	D	402	MES	C8-S	-7.87	1.66	1.77
5	D	404	MES	C8-S	-7.86	1.66	1.77
5	A	402	MES	C8-S	-7.73	1.66	1.77
5	B	402	MES	C8-S	-7.72	1.66	1.77
5	C	403	MES	C8-S	-7.72	1.66	1.77
5	F	402	MES	C8-S	-7.67	1.66	1.77
5	F	403	MES	C8-S	-7.65	1.66	1.77
5	D	403	MES	C8-S	-7.40	1.67	1.77

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	403	MES	C5-N4-C3	5.00	119.61	108.84
5	F	402	MES	O1S-S-C8	3.41	111.87	106.73
5	C	403	MES	C8-C7-N4	-3.14	104.23	112.39
5	B	402	MES	C8-C7-N4	-2.99	104.62	112.39
5	E	402	MES	C8-C7-N4	-2.91	104.82	112.39
5	F	403	MES	C3-N4-C7	2.88	120.03	112.01
5	D	403	MES	C7-N4-C3	2.80	118.70	111.24
5	A	402	MES	C3-N4-C7	2.73	119.62	112.01
5	D	403	MES	C2-C3-N4	-2.69	106.03	110.12
5	D	403	MES	C7-N4-C5	2.65	118.31	111.24
5	D	402	MES	C3-N4-C7	2.59	119.23	112.01
5	A	402	MES	C8-C7-N4	-2.57	104.08	111.40
5	F	402	MES	C8-C7-N4	-2.51	105.87	112.39
5	F	403	MES	C8-C7-N4	-2.51	104.25	111.40
5	D	404	MES	C8-C7-N4	-2.46	104.39	111.40
5	C	402	MES	O2S-S-C8	2.35	110.28	106.73
5	F	402	MES	O3S-S-C8	2.30	110.50	106.00
5	E	403	MES	O3S-S-C8	2.17	110.26	106.00
5	F	403	MES	O3S-S-C8	2.16	110.24	106.00
5	D	403	MES	C6-C5-N4	-2.11	106.91	110.12
5	D	403	MES	O1S-S-C8	2.11	109.91	106.73
5	A	402	MES	O1S-S-C8	2.07	109.86	106.73
5	D	402	MES	O1S-S-C8	2.07	109.86	106.73
5	C	404	MES	O1S-S-C8	2.03	109.80	106.73
5	E	402	MES	O1S-S-C8	2.02	109.77	106.73
5	C	403	MES	O3S-S-C8	2.01	109.94	106.00

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	402	MES	C8-C7-N4-C3
5	D	402	MES	C7-C8-S-O2S
5	D	402	MES	C7-C8-S-O3S
5	D	403	MES	C8-C7-N4-C3
5	D	403	MES	C8-C7-N4-C5
5	D	404	MES	C7-C8-S-O1S
5	D	404	MES	C7-C8-S-O3S
5	C	402	MES	C7-C8-S-O1S
5	C	402	MES	C7-C8-S-O2S
5	C	402	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
5	C	403	MES	C7-C8-S-O1S
5	C	403	MES	C7-C8-S-O3S
5	C	404	MES	C7-C8-S-O2S
5	C	404	MES	C7-C8-S-O3S
5	F	403	MES	C8-C7-N4-C3
5	D	404	MES	C8-C7-N4-C5
5	E	402	MES	C7-C8-S-O3S
5	F	402	MES	C7-C8-S-O3S
5	D	404	MES	C6-C5-N4-C7
5	B	402	MES	C7-C8-S-O3S
5	D	404	MES	C5-C6-O1-C2
5	C	404	MES	C7-C8-S-O1S
5	B	402	MES	C7-C8-S-O1S
5	B	402	MES	C7-C8-S-O2S
5	D	402	MES	C7-C8-S-O1S
5	D	404	MES	C7-C8-S-O2S
5	C	403	MES	C7-C8-S-O2S
5	E	402	MES	C7-C8-S-O1S
5	E	402	MES	C7-C8-S-O2S
5	F	402	MES	C7-C8-S-O1S
5	F	402	MES	C7-C8-S-O2S
5	F	403	MES	N4-C7-C8-S
5	B	402	MES	N4-C7-C8-S
5	F	402	MES	N4-C7-C8-S

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	403	MES	3	0
5	F	403	MES	1	0
5	E	402	MES	4	0
5	F	402	MES	2	0
5	D	404	MES	2	0
5	D	402	MES	3	0

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 ⓘ

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	324/324 (100%)	-0.22	10 (3%)	51	51	11, 20, 46, 95	5 (1%)
2	B	322/322 (100%)	-0.31	9 (2%)	55	54	8, 18, 41, 74	11 (3%)
2	D	322/322 (100%)	-0.31	6 (1%)	66	66	8, 19, 44, 86	7 (2%)
2	E	322/322 (100%)	-0.35	6 (1%)	66	66	7, 17, 44, 89	6 (1%)
2	F	322/322 (100%)	-0.46	7 (2%)	62	62	7, 15, 41, 91	12 (3%)
3	C	319/319 (100%)	-0.46	6 (1%)	66	66	7, 15, 38, 110	8 (2%)
All	All	1931/1931 (100%)	-0.35	44 (2%)	61	61	7, 17, 43, 110	49 (2%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1	VAL	9.3
2	F	81	VAL	5.0
2	D	1	VAL	4.8
1	A	81	VAL	4.6
1	A	3	LEU	4.3
1	A	-1	HIS	4.3
3	C	4	THR	4.2
2	D	80	PRO	4.1
2	B	1	VAL	4.1
2	D	81	VAL	4.0
2	D	79	ALA	3.9
2	E	2	PRO	3.8
2	E	0	HIS	3.6
2	F	20	PRO	3.5
2	E	81	VAL	3.5
3	C	5	PHE	3.3
2	F	1	VAL	3.3
1	A	4	THR	3.2
2	B	79	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	3.1
2	D	0	HIS	3.1
3	C	81	VAL	3.1
3	C	3	LEU	3.1
1	A	80	PRO	3.0
2	F	0	HIS	3.0
2	B	81	VAL	2.9
2	F	21	ARG	2.9
2	B	2	PRO	2.7
3	C	19	THR	2.6
2	B	4	THR	2.5
2	B	0	HIS	2.5
2	D	10	GLU	2.4
2	E	82	GLU	2.4
2	B	80	PRO	2.4
1	A	79	ALA	2.3
1	A	9	PHE	2.3
3	C	224	LYS	2.3
2	B	3	LEU	2.3
2	F	79	ALA	2.2
2	E	3	LEU	2.2
1	A	221	ASP	2.0
1	A	223	GLU	2.0
2	B	222	LEU	2.0
2	F	3	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
5	MES	C	404	6/12	0.72	0.24	67,84,86,87	0
5	MES	D	404	11/12	0.75	0.25	64,67,94,99	1
5	MES	E	403	6/12	0.75	0.17	46,59,65,70	0
5	MES	F	403	8/12	0.75	0.18	42,82,91,93	0
5	MES	E	402	7/12	0.77	0.19	80,84,94,95	0
5	MES	A	402	8/12	0.80	0.17	45,57,64,69	0
5	MES	C	403	7/12	0.86	0.15	52,57,60,69	0
6	SO4	A	403	5/5	0.86	0.12	51,65,65,69	0
5	MES	D	403	12/12	0.88	0.15	41,60,64,66	0
4	NA	E	401	1/1	0.88	0.09	31,31,31,31	0
5	MES	D	402	8/12	0.89	0.13	21,38,49,51	8
7	FMT	B	404	3/3	0.89	0.14	50,50,51,54	0
5	MES	B	402	7/12	0.90	0.12	35,47,56,56	0
5	MES	B	403	5/12	0.91	0.11	40,42,50,65	0
4	NA	A	401	1/1	0.91	0.07	35,35,35,35	0
5	MES	F	402	7/12	0.91	0.13	38,44,50,52	0
5	MES	C	402	6/12	0.93	0.11	28,33,34,43	0
4	NA	B	401	1/1	0.94	0.08	26,26,26,26	0
4	NA	D	401	1/1	0.95	0.05	31,31,31,31	0
4	NA	F	401	1/1	0.98	0.03	16,16,16,16	0
4	NA	C	401	1/1	0.98	0.03	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.