Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:30 am BST

PDB ID	:	6HFZ
Title	:	Crystal structure of a two-domain esterase (CEX) active on acetylated mannans
Authors	:	Michalak, L.; La Rosa, S.L.; Rohr, A.K.; Aachmann, F.L.; Westereng, B.
Deposited on	:	2018-08-22
Resolution	:	1.75 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 ①) were used in the production of this report:

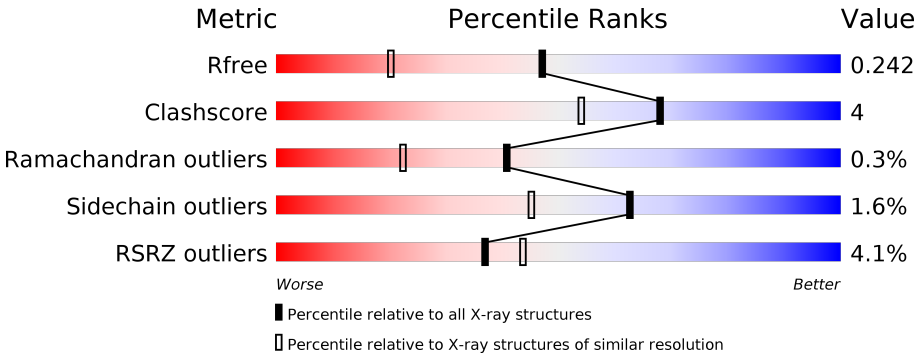
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 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 <=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	378	90% 7%
1	B	378	% 88% 8%
1	C	378	% 90% 7%
1	D	378	13% 82% 13%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	C	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12466 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 GDSL-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	Se	0	1	0
			2898	1829	496	563	5	5			
1	B	368	Total	C	N	O	S	Se	0	1	0
			2914	1841	500	564	5	4			
1	C	371	Total	C	N	O	S	Se	0	0	0
			2916	1836	500	571	5	4			
1	D	364	Total	C	N	O	S	Se	0	1	0
			2873	1813	490	560	6	4			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP C7G6F8
A	373	ALA	-	expression tag	UNP C7G6F8
A	374	HIS	-	expression tag	UNP C7G6F8
A	375	HIS	-	expression tag	UNP C7G6F8
A	376	HIS	-	expression tag	UNP C7G6F8
A	377	HIS	-	expression tag	UNP C7G6F8
A	378	HIS	-	expression tag	UNP C7G6F8
B	1	MSE	-	initiating methionine	UNP C7G6F8
B	373	ALA	-	expression tag	UNP C7G6F8
B	374	HIS	-	expression tag	UNP C7G6F8
B	375	HIS	-	expression tag	UNP C7G6F8
B	376	HIS	-	expression tag	UNP C7G6F8
B	377	HIS	-	expression tag	UNP C7G6F8
B	378	HIS	-	expression tag	UNP C7G6F8
C	1	MSE	-	initiating methionine	UNP C7G6F8
C	373	ALA	-	expression tag	UNP C7G6F8
C	374	HIS	-	expression tag	UNP C7G6F8
C	375	HIS	-	expression tag	UNP C7G6F8
C	376	HIS	-	expression tag	UNP C7G6F8
C	377	HIS	-	expression tag	UNP C7G6F8
C	378	HIS	-	expression tag	UNP C7G6F8

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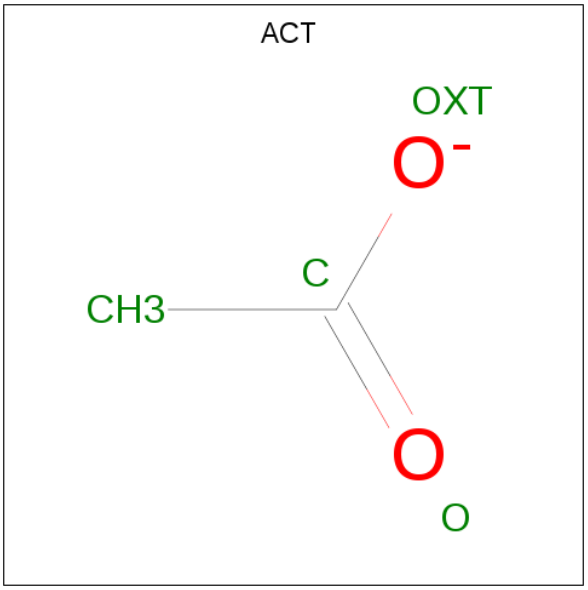
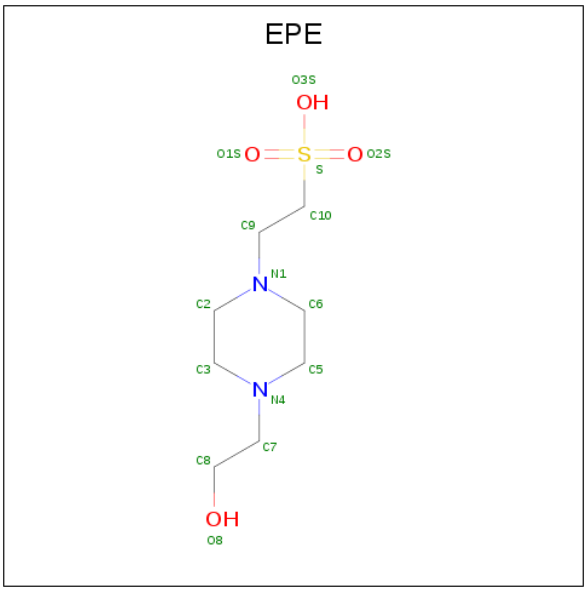
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	-	initiating methionine	UNP C7G6F8
D	373	ALA	-	expression tag	UNP C7G6F8
D	374	HIS	-	expression tag	UNP C7G6F8
D	375	HIS	-	expression tag	UNP C7G6F8
D	376	HIS	-	expression tag	UNP C7G6F8
D	377	HIS	-	expression tag	UNP C7G6F8
D	378	HIS	-	expression tag	UNP C7G6F8

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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	C	1	Total C O 4 2 2	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is water.

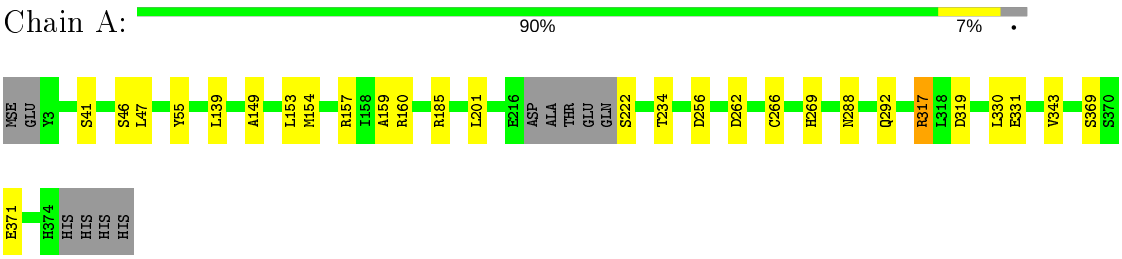
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	274	Total	O	0	0
			274	274		
4	B	210	Total	O	0	0
			210	210		
4	C	235	Total	O	0	0
			235	235		
4	D	89	Total	O	0	0
			89	89		

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.

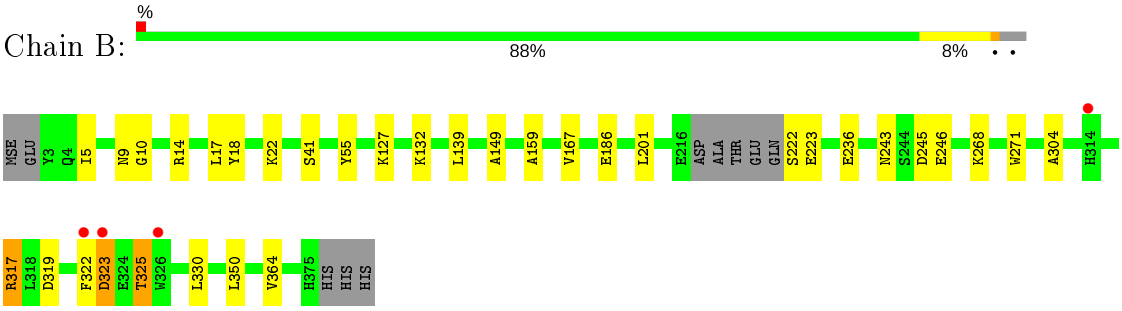
- Molecule 1: GDSL-like protein

Chain A:



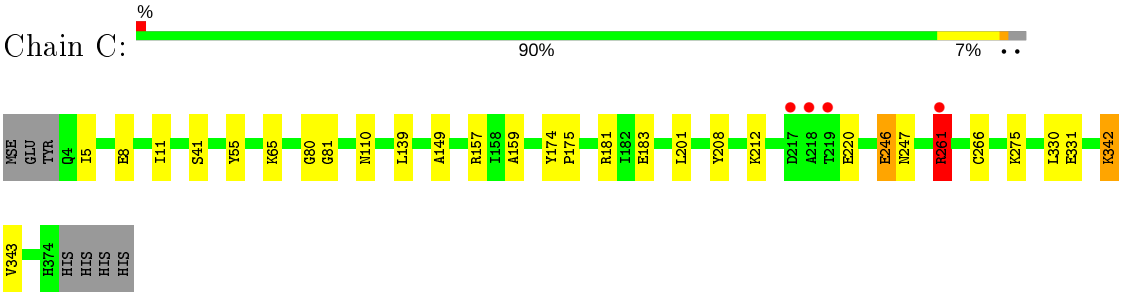
- Molecule 1: GDSL-like protein

Chain B:



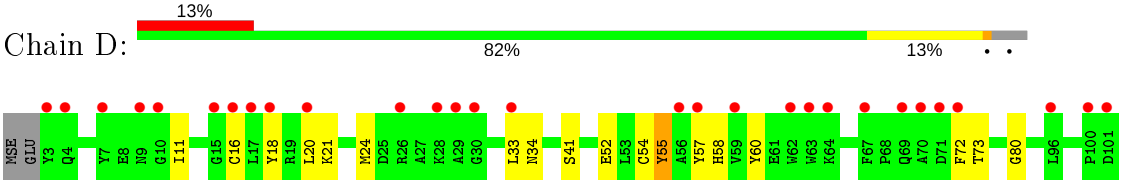
- Molecule 1: GDSL-like protein

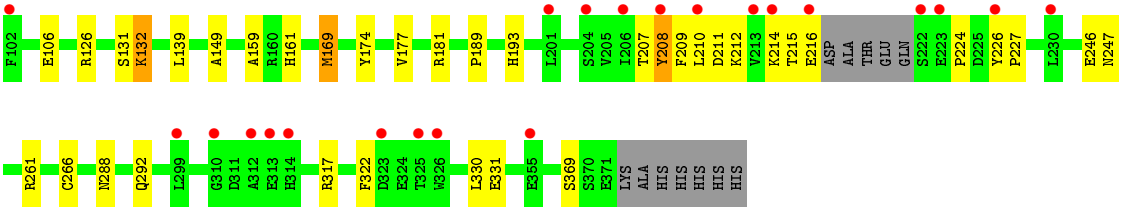
Chain C:



- Molecule 1: GDSL-like protein

Chain D:




F102
E106
R126
S131
K132
L139
A149
A159
R160
H161
M169
Y174
V177
R181
P189
H193
L201
S204
V205
I206
T207
Y208
F209
L210
D211
K212
V213
K214
T215
E216
ASP
ALA
THR
GLU
GLN
S222
E223
P224
D225
Y226
P227
L230
E246
N247
R261
C266
N288
Q292
L299
G310
D311
A312
E313
H314
R317
F322
D323
E324
T325
W326
L330
E331
E355
S369
S370
E371
LYS
ALA
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.12Å 136.52Å 85.13Å 90.00° 115.09° 90.00°	Depositor
Resolution (Å)	47.87 – 1.75 47.82 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.87-1.75) 99.9 (47.82-1.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.190 , 0.232 0.200 , 0.242	Depositor DCC
R_{free} test set	7628 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12466	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EPE, ACT

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	0.62	0/2959	0.76	1/4008 (0.0%)
1	B	0.59	0/2978	0.74	0/4036
1	C	0.62	1/2977 (0.0%)	0.77	0/4035
1	D	0.53	0/2933	0.74	2/3975 (0.1%)
All	All	0.59	1/11847 (0.0%)	0.75	3/16054 (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	A	0	2
1	B	0	2
1	C	0	3
1	D	0	3
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	331	GLU	CD-OE2	5.16	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	169	MSE	CG-SE-CE	-7.67	82.03	98.90
1	A	160	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	D	169	MSE	N-CA-CB	5.38	120.28	110.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	ARG	Sidechain
1	A	317	ARG	Sidechain
1	B	317	ARG	Sidechain
1	B	325	THR	Peptide
1	C	157	ARG	Sidechain
1	C	181	ARG	Sidechain
1	C	261	ARG	Sidechain
1	D	181	ARG	Sidechain
1	D	214	LYS	Peptide
1	D	317	ARG	Sidechain

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	2898	0	2805	16	0
1	B	2914	0	2813	18	1
1	C	2916	0	2819	21	1
1	D	2873	0	2780	33	0
2	A	4	0	3	1	0
2	B	4	0	3	1	0
2	C	4	0	3	7	0
3	A	15	0	18	1	0
3	B	15	0	18	0	0
3	D	15	0	18	0	0
4	A	274	0	0	3	0
4	B	210	0	0	3	0
4	C	235	0	0	4	0
4	D	89	0	0	5	0
All	All	12466	0	11280	86	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (86) 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:C:110:ASN:HD21	2:C:401:ACT:H2	0.97	1.12
1:C:41:SER:H	2:C:401:ACT:H3	1.20	1.01
1:C:110:ASN:ND2	2:C:401:ACT:H2	1.83	0.92
1:C:81:GLY:H	2:C:401:ACT:H1	1.34	0.91
1:D:20:LEU:CB	4:D:514:HOH:O	2.25	0.84
1:D:20:LEU:HB2	4:D:514:HOH:O	1.77	0.83
1:B:186:GLU:OE2	4:B:501:HOH:O	2.01	0.78
1:C:343:VAL:HG12	4:C:661:HOH:O	1.89	0.73
1:D:169:MSE:HE2	1:D:169:MSE:N	2.05	0.71
1:C:41:SER:N	2:C:401:ACT:H3	2.02	0.70
1:D:169:MSE:CA	1:D:169:MSE:HE2	2.26	0.65
1:D:57:TYR:O	1:D:60:TYR:N	2.29	0.65
1:C:81:GLY:H	2:C:401:ACT:CH3	2.05	0.65
1:C:81:GLY:N	2:C:401:ACT:H1	2.11	0.65
1:A:262:ASP:HB2	4:A:714:HOH:O	1.98	0.63
1:D:207:THR:O	1:D:210:LEU:N	2.32	0.62
1:C:220:GLU:HG2	4:C:591:HOH:O	2.00	0.62
1:D:54[A]:CYS:SG	1:D:55:TYR:N	2.73	0.60
1:A:234:THR:HG22	1:A:371:GLU:HG3	1.83	0.60
1:A:41:SER:OG	2:A:401:ACT:C	2.51	0.59
1:C:342:LYS:NZ	4:C:501:HOH:O	2.27	0.59
1:D:21:LYS:HA	4:D:510:HOH:O	2.03	0.57
1:A:343:VAL:HG12	4:A:646:HOH:O	2.04	0.57
1:D:126:ARG:CZ	1:D:226:TYR:OH	2.52	0.57
1:C:8:GLU:OE2	1:C:208:TYR:OH	2.06	0.57
1:C:139:LEU:HD12	1:C:159:ALA:HB2	1.85	0.57
1:D:139:LEU:HD12	1:D:159:ALA:HB2	1.86	0.57
1:A:154:MSE:HE1	1:A:157:ARG:NH1	2.20	0.56
1:C:275:LYS:HG3	4:C:729:HOH:O	2.05	0.55
1:C:246:GLU:O	1:C:247:ASN:HB2	2.09	0.53
1:D:169:MSE:HA	1:D:169:MSE:HE2	1.90	0.53
1:B:245:ASP:OD2	1:B:246:GLU:O	2.27	0.53
1:D:288:ASN:HB2	1:D:369:SER:HB2	1.91	0.52
1:D:33:LEU:O	1:D:72:PHE:HA	2.09	0.52
1:D:207:THR:O	1:D:208:TYR:C	2.48	0.52
1:B:243:ASN:HA	1:B:271:TRP:CZ2	2.45	0.51
1:B:268:LYS:HE2	4:B:509:HOH:O	2.10	0.50
1:C:11:ILE:CD1	1:C:212:LYS:HE3	2.42	0.50
1:B:18:TYR:CE2	1:B:22:LYS:HE2	2.48	0.49
1:D:34:ASN:OD1	1:D:73:THR:HB	2.13	0.49
1:B:222:SER:N	4:B:506:HOH:O	2.46	0.48
1:B:5:ILE:CD1	1:B:201:LEU:HD22	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ALA:HB2	1:B:350:LEU:HD23	1.95	0.48
1:B:323:ASP:N	1:B:323:ASP:OD1	2.39	0.48
1:C:5:ILE:HD12	1:C:201:LEU:HD11	1.95	0.48
1:A:317:ARG:HD3	1:A:319:ASP:HB2	1.94	0.47
1:A:139:LEU:HD12	1:A:159:ALA:HB2	1.96	0.47
1:B:330:LEU:CD1	1:B:364:VAL:HG21	2.45	0.47
1:D:246:GLU:O	1:D:247:ASN:HB2	2.14	0.47
1:D:21:LYS:NZ	1:D:216:GLU:O	2.36	0.46
1:D:131:SER:O	1:D:132:LYS:C	2.54	0.46
1:D:41:SER:HB3	1:D:80:GLY:HA2	1.97	0.46
1:A:269:HIS:HD2	4:A:514:HOH:O	1.99	0.46
1:D:16:CYS:SG	1:D:224:PRO:HD3	2.56	0.45
1:A:266:CYS:HB2	1:A:330:LEU:HD22	1.99	0.45
1:D:292:GLN:HA	1:D:331:GLU:O	2.18	0.44
1:D:174:TYR:O	1:D:177:VAL:N	2.51	0.44
1:D:161:HIS:O	1:D:227:PRO:HG3	2.17	0.44
1:D:20:LEU:HB3	4:D:514:HOH:O	2.01	0.44
1:B:246:GLU:H	1:B:246:GLU:HG3	1.63	0.44
1:D:52:GLU:HA	1:D:57:TYR:CD2	2.52	0.43
1:B:14:ARG:NH2	1:B:17:LEU:HD12	2.33	0.43
1:A:46:SER:HA	1:A:47:LEU:HA	1.86	0.43
1:B:139:LEU:HD12	1:B:159:ALA:HB2	2.01	0.43
1:B:317:ARG:NH1	1:B:319:ASP:OD2	2.52	0.43
1:B:41:SER:OG	2:B:401:ACT:C	2.67	0.42
1:A:292:GLN:HA	1:A:331:GLU:O	2.20	0.42
1:B:127:LYS:CE	1:B:236:GLU:O	2.67	0.42
1:A:153:LEU:HD23	1:A:154:MSE:CE	2.48	0.42
1:C:149:ALA:HB2	1:D:149:ALA:HB2	2.00	0.42
1:D:266:CYS:HB2	1:D:330:LEU:HD22	2.02	0.42
1:A:149:ALA:HB2	1:B:149:ALA:HB2	2.01	0.42
1:C:41:SER:HB3	1:C:80:GLY:HA2	2.02	0.42
1:D:207:THR:O	1:D:209:PHE:N	2.53	0.42
1:C:246:GLU:O	1:C:247:ASN:CB	2.68	0.41
1:A:343:VAL:O	1:A:343:VAL:HG13	2.20	0.41
1:D:34:ASN:OD1	1:D:73:THR:CB	2.68	0.41
1:C:174:TYR:HB3	1:C:175:PRO:HD3	2.01	0.41
1:A:256:ASP:OD1	3:A:402:EPE:H31	2.20	0.41
1:D:24:MSE:SE	4:D:510:HOH:O	2.88	0.41
1:A:288:ASN:HB2	1:A:369:SER:HB2	2.03	0.41
1:C:266:CYS:HB2	1:C:330:LEU:HD22	2.03	0.41
1:B:10:GLY:O	1:B:167:VAL:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:PRO:HD2	1:D:193:HIS:O	2.21	0.40
1:D:57:TYR:O	1:D:58:HIS:C	2.60	0.40
1:D:11:ILE:CD1	1:D:212:LYS:HE3	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ASN:OD1	1:C:261:ARG:NH1[2_456]	2.19	0.01

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	364/378 (96%)	355 (98%)	9 (2%)	0	100 100
1	B	365/378 (97%)	348 (95%)	17 (5%)	0	100 100
1	C	369/378 (98%)	357 (97%)	12 (3%)	0	100 100
1	D	361/378 (96%)	335 (93%)	22 (6%)	4 (1%)	14 3
All	All	1459/1512 (96%)	1395 (96%)	60 (4%)	4 (0%)	41 22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	132	LYS
1	D	18	TYR
1	D	211	ASP
1	D	208	TYR

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	314/318 (99%)	311 (99%)	3 (1%)	76	63
1	B	315/318 (99%)	309 (98%)	6 (2%)	57	37
1	C	316/318 (99%)	310 (98%)	6 (2%)	57	37
1	D	312/318 (98%)	307 (98%)	5 (2%)	62	45
All	All	1257/1272 (99%)	1237 (98%)	20 (2%)	62	45

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	TYR
1	A	201	LEU
1	A	222	SER
1	B	55	TYR
1	B	132	LYS
1	B	223	GLU
1	B	322	PHE
1	B	323	ASP
1	B	325	THR
1	C	55	TYR
1	C	65	LYS
1	C	183	GLU
1	C	246	GLU
1	C	261	ARG
1	C	342	LYS
1	D	55	TYR
1	D	106	GLU
1	D	215	THR
1	D	261	ARG
1	D	322	PHE

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

Mol	Chain	Res	Type
1	A	4	GLN
1	A	269	HIS
1	C	9	ASN
1	C	110	ASN
1	C	221	GLN
1	D	142	ASN
1	D	241	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

6 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	$\#\|Z\| > 2$
3	EPE	D	401	-	15,15,15	2.35	1 (6%)	18,20,20	1.49	3 (16%)
2	ACT	C	401	-	1,3,3	3.06	1 (100%)	0,3,3	0.00	-
2	ACT	B	401	-	1,3,3	3.82	1 (100%)	0,3,3	0.00	-
2	ACT	A	401	-	1,3,3	0.95	0	0,3,3	0.00	-
3	EPE	A	402	-	15,15,15	1.52	1 (6%)	18,20,20	1.85	2 (11%)
3	EPE	B	402	-	15,15,15	1.86	1 (6%)	18,20,20	1.55	3 (16%)

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
3	EPE	D	401	-	-	3/9/19/19	0/1/1/1
3	EPE	A	402	-	-	0/9/19/19	0/1/1/1
3	EPE	B	402	-	-	0/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	EPE	C10-S	-8.96	1.64	1.77
3	B	402	EPE	C10-S	-6.63	1.68	1.77
3	A	402	EPE	C10-S	-5.32	1.69	1.77
2	B	401	ACT	CH3-C	3.82	1.53	1.48
2	C	401	ACT	CH3-C	-3.06	1.44	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	402	EPE	O2S-S-C10	5.72	113.80	106.92
3	D	401	EPE	O2S-S-C10	3.68	111.35	106.92
3	B	402	EPE	C3-C2-N1	-3.28	103.90	110.64
3	B	402	EPE	C9-N1-C6	2.94	118.75	111.23
3	D	401	EPE	C8-C7-N4	-2.36	104.92	113.40
3	A	402	EPE	O3S-S-C10	-2.29	102.07	105.77
3	B	402	EPE	C6-C5-N4	2.11	114.97	110.64
3	D	401	EPE	O3S-S-C10	2.09	109.15	105.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	EPE	N4-C7-C8-O8
3	D	401	EPE	C8-C7-N4-C3
3	D	401	EPE	C8-C7-N4-C5

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	ACT	7	0
2	B	401	ACT	1	0
2	A	401	ACT	1	0
3	A	402	EPE	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, 95^{th} 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	363/378 (96%)	-0.14	0 100 100	18, 26, 43, 65	0
1	B	364/378 (96%)	0.01	4 (1%) 80 86	17, 30, 56, 90	0
1	C	367/378 (97%)	0.05	4 (1%) 80 86	19, 30, 51, 84	0
1	D	360/378 (95%)	0.90	51 (14%) 2 3	25, 47, 80, 136	0
All	All	1454/1512 (96%)	0.20	59 (4%) 37 44	17, 32, 63, 136	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	222	SER	14.5
1	D	3	TYR	7.1
1	B	326[A]	TRP	5.4
1	B	323	ASP	5.3
1	D	210	LEU	5.2
1	D	18	TYR	5.1
1	D	4	GLN	5.0
1	D	102	PHE	4.9
1	D	223	GLU	4.7
1	D	33	LEU	4.6
1	D	214	LYS	4.4
1	D	67	PHE	4.4
1	D	57	TYR	4.2
1	B	314	HIS	3.9
1	D	355	GLU	3.7
1	D	314	HIS	3.6
1	D	208	TYR	3.4
1	D	15	GLY	3.4
1	D	17	LEU	3.3
1	D	310	GLY	3.3
1	D	201	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	9	ASN	3.2
1	D	29	ALA	3.2
1	D	28	LYS	3.1
1	D	64	LYS	3.1
1	C	218	ALA	3.0
1	D	70	ALA	3.0
1	D	312	ALA	2.9
1	D	16	CYS	2.9
1	C	261	ARG	2.9
1	D	313	GLU	2.9
1	D	71	ASP	2.9
1	D	213	VAL	2.9
1	C	219	THR	2.8
1	D	204	SER	2.7
1	D	323	ASP	2.7
1	D	72	PHE	2.7
1	C	217	ASP	2.6
1	D	96	LEU	2.6
1	D	7	TYR	2.6
1	D	226	TYR	2.5
1	D	56	ALA	2.5
1	D	63	TRP	2.5
1	D	326	TRP	2.5
1	D	30	GLY	2.5
1	D	69	GLN	2.5
1	D	26	ARG	2.3
1	D	230	LEU	2.3
1	D	206	ILE	2.3
1	D	100	PRO	2.3
1	D	325	THR	2.3
1	D	20	LEU	2.2
1	D	101	ASP	2.2
1	D	216	GLU	2.1
1	D	10	GLY	2.1
1	B	322	PHE	2.1
1	D	299	LEU	2.1
1	D	59	VAL	2.0
1	D	62	TRP	2.0

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

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

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, 95^{th} 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	ACT	C	401	4/4	0.72	0.25	22,33,35,41	0
2	ACT	B	401	4/4	0.94	0.10	27,29,30,31	0
3	EPE	B	402	15/15	0.94	0.14	42,46,54,54	0
2	ACT	A	401	4/4	0.96	0.09	25,31,31,32	0
3	EPE	A	402	15/15	0.96	0.11	36,44,48,50	0
3	EPE	D	401	15/15	0.96	0.10	40,43,50,52	0

6.5 Other polymers (i)

There are no such residues in this entry.