



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 02:46 am BST

PDB ID : 3LMV
Title : D-Tyr-tRNA(Tyr) Deacylase from plasmodium falciparum in complex with hepes
Authors : Manickam, Y.; Khan, S.; Bhatt, T.K.; Sharma, A.
Deposited on : 2010-02-01
Resolution : 2.83 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 : 1.8.5 (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

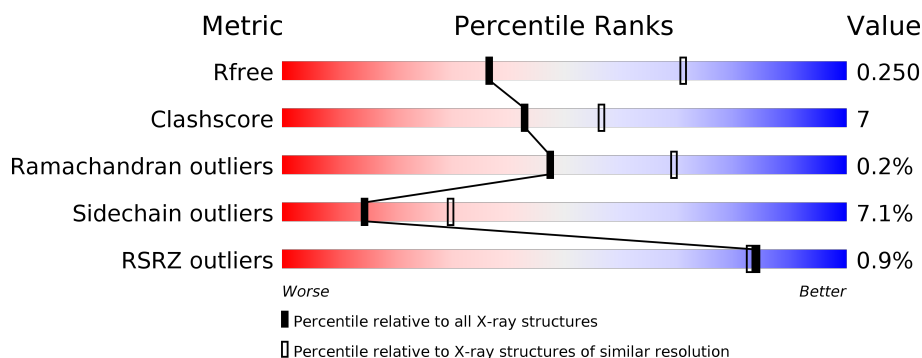
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 $\leq 5\%$. 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	164	<div> <div style="width: 4%;"></div> <div style="width: 77%;"></div> <div style="width: 13%;"></div> <div style="width: 7%;"></div> </div>
1	B	164	<div> <div style="width: 76%;"></div> <div style="width: 14%;"></div> <div style="width: 7%;"></div> </div>
1	C	164	<div> <div style="width: 74%;"></div> <div style="width: 16%;"></div> <div style="width: 8%;"></div> </div>
1	D	164	<div> <div style="width: 79%;"></div> <div style="width: 11%;"></div> <div style="width: 9%;"></div> </div>
1	E	164	<div> <div style="width: 4%;"></div> <div style="width: 70%;"></div> <div style="width: 10%;"></div> <div style="width: 19%;"></div> </div>
1	F	164	<div> <div style="width: 70%;"></div> <div style="width: 16%;"></div> <div style="width: 13%;"></div> </div>

2 Entry composition [i](#)

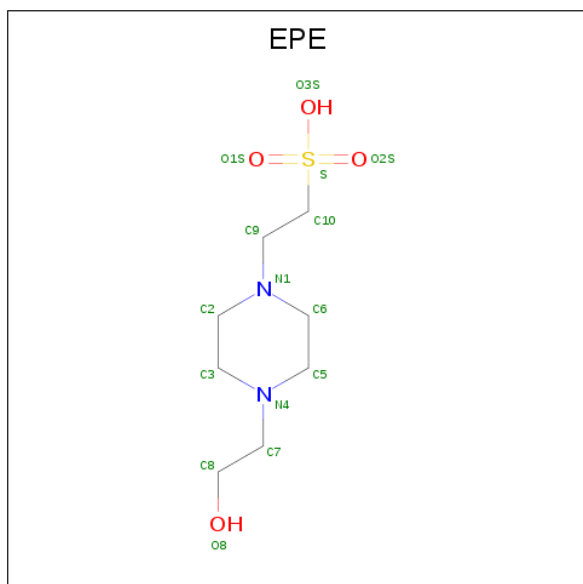
There are 3 unique types of molecules in this entry. The entry contains 7047 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-tyrosyl-tRNA(Tyr) deacylase.

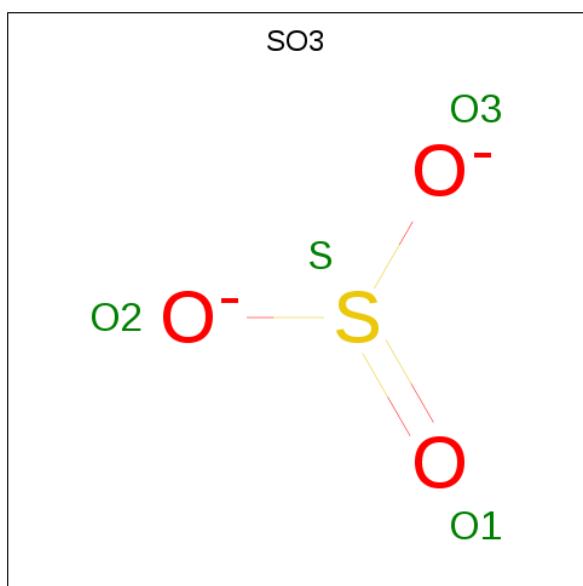
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1192	771	198	220	3			
1	B	152	Total	C	N	O	S	1	0	0
			1193	768	198	224	3			
1	C	151	Total	C	N	O	S	0	0	0
			1220	785	206	226	3			
1	D	150	Total	C	N	O	S	1	0	0
			1185	766	201	215	3			
1	E	133	Total	C	N	O	S	0	0	0
			1032	671	171	187	3			
1	F	143	Total	C	N	O	S	0	0	0
			1138	737	189	209	3			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 3 is SULFITE ION (three-letter code: SO3) (formula: O₃S).

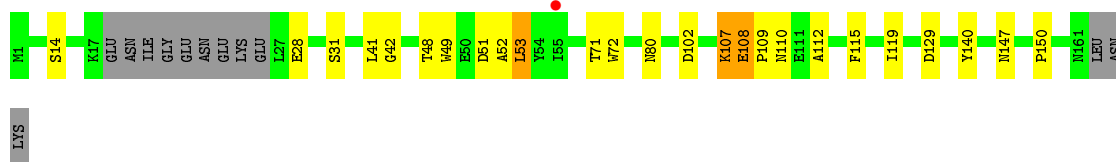


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			4	3	1		
3	B	1	Total	O	S	0	0
			4	3	1		
3	F	1	Total	O	S	1	0
			4	3	1		

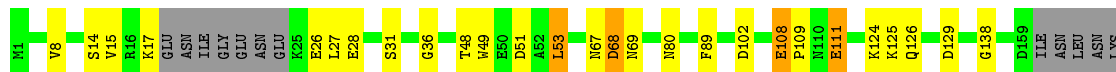
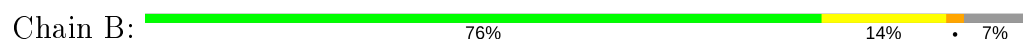
3 Residue-property plots [i](#)

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.

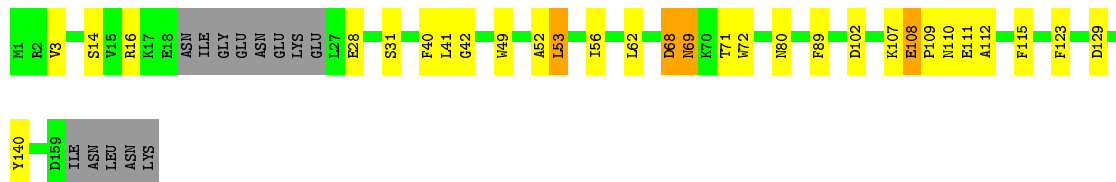
- Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase



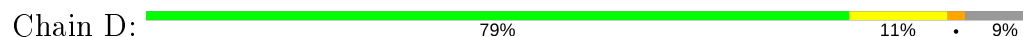
- Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase



- Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase

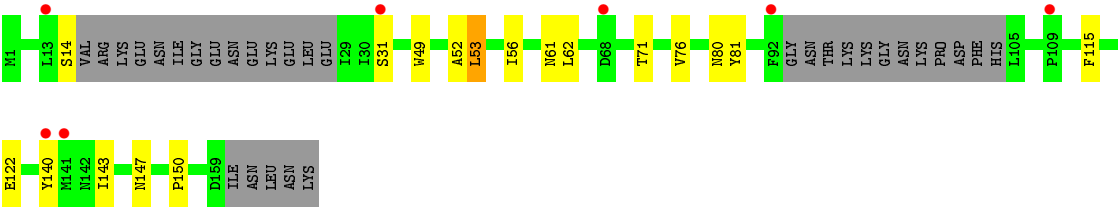


- Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase

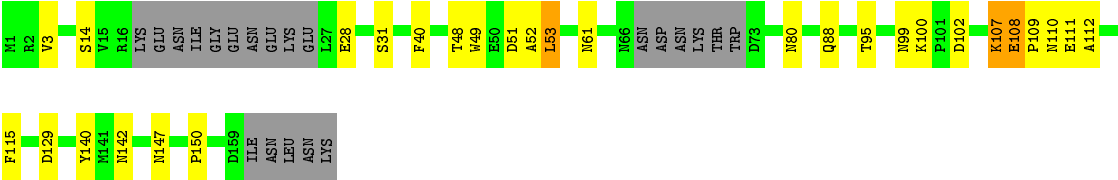


- Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase





● Molecule 1: D-tyrosyl-tRNA(Tyr) deacylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.65Å 52.95Å 89.68Å 75.40° 74.20° 86.10°	Depositor
Resolution (Å)	29.24 – 2.83 49.70 – 2.83	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.24-2.83) 96.8 (49.70-2.83)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.5 _2	Depositor
R, R_{free}	0.207 , 0.251 0.204 , 0.250	Depositor DCC
R_{free} test set	1043 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7047	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO3, EPE

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	0.56	0/1215	0.59	0/1651
1	B	0.63	0/1213	0.59	0/1646
1	C	0.60	0/1243	0.58	0/1683
1	D	0.59	0/1207	0.56	0/1637
1	E	0.59	0/1051	0.56	0/1431
1	F	0.59	2/1158 (0.2%)	0.59	0/1567
All	All	0.59	2/7087 (0.0%)	0.58	0/9615

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	61	ASN	CG-OD1	5.31	1.35	1.24
1	F	142	ASN	CG-OD1	5.05	1.35	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1192	0	1142	12	0
1	B	1193	0	1134	22	1
1	C	1220	0	1196	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1185	0	1147	11	1
1	E	1032	0	970	14	0
1	F	1138	0	1118	18	0
2	A	15	0	17	0	0
2	B	30	0	34	7	0
2	C	15	0	17	1	0
2	D	15	0	17	0	0
3	B	8	0	0	0	0
3	F	4	0	0	0	0
All	All	7047	0	6792	94	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 7.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:GLU:OE2	1:F:110:ASN:HB2	1.82	0.78
1:C:108:GLU:OE2	1:C:110:ASN:HB2	1.83	0.78
1:A:108:GLU:OE2	1:A:110:ASN:HB2	1.83	0.77
1:B:125:LYS:CA	1:B:125:LYS:O	2.39	0.71
1:B:89:PHE:CE2	2:B:165:EPE:H22	2.26	0.70
1:C:108:GLU:OE1	1:C:111:GLU:HG3	1.92	0.70
1:B:125:LYS:O	1:B:126:GLN:N	2.25	0.69
1:C:68:ASP:O	1:C:69:ASN:HB3	1.92	0.69
1:B:89:PHE:CE2	2:B:165:EPE:H101	2.31	0.66
1:D:66:ASN:OD1	1:D:71:THR:HA	1.95	0.65
1:B:17:LYS:H	1:B:26:GLU:CB	2.10	0.64
1:B:125:LYS:CA	1:B:126:GLN:N	2.62	0.63
1:B:89:PHE:HE2	2:B:165:EPE:H22	1.63	0.63
1:B:67:ASN:C	1:B:69:ASN:H	2.03	0.60
1:B:89:PHE:HE2	2:B:165:EPE:H101	1.65	0.60
1:B:138:GLY:HA2	2:B:165:EPE:H102	1.84	0.60
1:C:68:ASP:O	1:C:68:ASP:CG	2.41	0.59
1:C:68:ASP:O	1:C:69:ASN:CB	2.54	0.55
1:C:108:GLU:HG2	1:C:109:PRO:HD2	1.90	0.54
1:B:108:GLU:HG2	1:B:109:PRO:HD2	1.87	0.54
1:F:108:GLU:HG2	1:F:109:PRO:HD2	1.90	0.54
1:A:108:GLU:HG2	1:A:109:PRO:HD2	1.91	0.53
1:A:71:THR:O	1:A:72:TRP:C	2.48	0.51
1:C:49:TRP:CD1	1:C:53:LEU:CD2	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:TRP:CD1	1:F:53:LEU:CD2	2.94	0.50
1:B:111:GLU:OE1	1:B:111:GLU:N	2.45	0.50
1:B:67:ASN:O	1:B:69:ASN:N	2.44	0.50
1:F:108:GLU:OE1	1:F:111:GLU:HG3	2.12	0.50
1:F:147:ASN:HB3	1:F:150:PRO:HB3	1.92	0.50
1:F:88:GLN:NE2	1:F:88:GLN:HA	2.26	0.50
1:B:108:GLU:OE1	1:B:111:GLU:CD	2.51	0.49
1:D:49:TRP:CD1	1:D:53:LEU:CD2	2.96	0.49
1:A:49:TRP:CD1	1:A:53:LEU:CD2	2.96	0.49
1:D:66:ASN:CG	1:D:71:THR:HA	2.32	0.49
1:B:15:VAL:O	1:B:27:LEU:HA	2.13	0.48
1:E:49:TRP:CD1	1:E:53:LEU:CD2	2.96	0.48
2:B:166:EPE:H101	2:B:166:EPE:H21	1.23	0.47
1:E:71:THR:O	1:F:100:LYS:NZ	2.44	0.47
1:E:61:ASN:HB3	1:F:99:ASN:ND2	2.30	0.47
1:A:52:ALA:HB2	1:A:115:PHE:CE2	2.50	0.47
1:E:52:ALA:HB2	1:E:115:PHE:CE2	2.50	0.47
1:E:143:ILE:CD1	1:F:150:PRO:HG3	2.45	0.46
1:A:107:LYS:HD3	1:A:112:ALA:HA	1.98	0.46
1:B:49:TRP:CD1	1:B:53:LEU:CD2	2.98	0.46
1:B:8:VAL:HG22	1:B:36:GLY:O	2.15	0.46
1:D:147:ASN:HB3	1:D:150:PRO:HB3	1.98	0.46
1:E:143:ILE:HD12	1:F:150:PRO:HG3	1.98	0.46
1:A:52:ALA:HB2	1:A:115:PHE:HE2	1.80	0.45
1:C:107:LYS:HD3	1:C:112:ALA:HA	1.98	0.45
1:E:140:TYR:C	1:E:140:TYR:CD2	2.88	0.45
1:C:52:ALA:HB2	1:C:115:PHE:CE2	2.50	0.45
1:A:147:ASN:HB3	1:A:150:PRO:HB3	1.99	0.45
1:B:67:ASN:C	1:B:69:ASN:N	2.69	0.45
2:B:166:EPE:H51	2:B:166:EPE:H81	1.68	0.45
1:A:52:ALA:HB1	1:A:119:ILE:HG12	1.98	0.45
1:B:48:THR:O	1:B:51:ASP:HB2	2.17	0.45
1:F:52:ALA:HB2	1:F:115:PHE:CE2	2.52	0.45
1:F:140:TYR:C	1:F:140:TYR:CD2	2.91	0.45
1:C:49:TRP:CD1	1:C:53:LEU:HD21	2.52	0.44
1:D:52:ALA:HB2	1:D:115:PHE:CE2	2.53	0.44
1:D:71:THR:O	1:D:72:TRP:C	2.56	0.44
1:F:107:LYS:HD3	1:F:112:ALA:HA	2.00	0.43
1:C:140:TYR:C	1:C:140:TYR:CD2	2.91	0.43
1:E:52:ALA:HB2	1:E:115:PHE:HE2	1.83	0.43
1:D:107:LYS:HD3	1:D:112:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:VAL:HA	1:C:40:PHE:O	2.19	0.42
1:E:147:ASN:HB3	1:E:150:PRO:HB3	2.01	0.42
1:B:108:GLU:HA	1:B:109:PRO:HD3	1.85	0.42
1:D:140:TYR:CD2	1:D:140:TYR:C	2.92	0.42
1:E:49:TRP:CD1	1:E:53:LEU:HD21	2.55	0.42
1:F:48:THR:O	1:F:51:ASP:HB2	2.20	0.42
1:E:56:ILE:HD13	1:E:122:GLU:HB3	2.01	0.42
1:E:62:LEU:HD21	1:F:95:THR:HB	2.00	0.42
1:E:62:LEU:HA	1:E:62:LEU:HD23	1.88	0.42
1:F:108:GLU:HA	1:F:109:PRO:HD3	1.85	0.42
1:C:71:THR:HB	1:C:72:TRP:CD1	2.55	0.42
1:D:49:TRP:CD1	1:D:53:LEU:HD21	2.55	0.42
1:C:52:ALA:HB2	1:C:115:PHE:HE2	1.85	0.42
1:A:140:TYR:C	1:A:140:TYR:CD2	2.92	0.41
1:B:108:GLU:OE1	1:B:111:GLU:OE2	2.38	0.41
1:C:108:GLU:HA	1:C:109:PRO:HD3	1.85	0.41
1:D:62:LEU:HD23	1:D:62:LEU:HA	1.88	0.41
1:C:62:LEU:HA	1:C:62:LEU:HD23	1.90	0.41
1:D:52:ALA:HB1	1:D:119:ILE:HG12	2.02	0.41
1:E:76:VAL:HG23	1:E:81:TYR:HB2	2.03	0.41
1:A:48:THR:O	1:A:51:ASP:HB2	2.20	0.41
1:B:53:LEU:HD13	1:B:53:LEU:HA	1.87	0.41
1:F:49:TRP:CD1	1:F:53:LEU:HD21	2.55	0.41
1:F:3:VAL:HA	1:F:40:PHE:O	2.20	0.41
1:C:53:LEU:HA	1:C:53:LEU:HD13	1.92	0.40
1:A:41:LEU:HD23	1:A:42:GLY:N	2.36	0.40
1:C:56:ILE:HG23	1:C:123:PHE:CD1	2.56	0.40
1:C:41:LEU:HD23	1:C:42:GLY:N	2.36	0.40
1:C:89:PHE:HE2	2:C:165:EPE:H101	1.86	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:124:LYS:NZ	1:D:32:GLU:OE1[1_665]	2.15	0.05

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	148/164 (90%)	138 (93%)	10 (7%)	0	100	100
1	B	146/164 (89%)	135 (92%)	10 (7%)	1 (1%)	22	42
1	C	147/164 (90%)	138 (94%)	8 (5%)	1 (1%)	22	42
1	D	144/164 (88%)	133 (92%)	11 (8%)	0	100	100
1	E	127/164 (77%)	119 (94%)	8 (6%)	0	100	100
1	F	137/164 (84%)	128 (93%)	9 (7%)	0	100	100
All	All	849/984 (86%)	791 (93%)	56 (7%)	2 (0%)	47	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	69	ASN
1	B	68	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	123/151 (82%)	114 (93%)	9 (7%)	14	29
1	B	123/151 (82%)	113 (92%)	10 (8%)	11	24
1	C	131/151 (87%)	121 (92%)	10 (8%)	13	28
1	D	123/151 (82%)	114 (93%)	9 (7%)	14	29
1	E	102/151 (68%)	98 (96%)	4 (4%)	32	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	121/151 (80%)	112 (93%)	9 (7%)	13	29
All	All	723/906 (80%)	672 (93%)	51 (7%)	14	30

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	28	GLU
1	A	31	SER
1	A	53	LEU
1	A	80	ASN
1	A	102	ASP
1	A	107	LYS
1	A	108	GLU
1	A	129	ASP
1	B	14	SER
1	B	28	GLU
1	B	31	SER
1	B	53	LEU
1	B	68	ASP
1	B	80	ASN
1	B	102	ASP
1	B	108	GLU
1	B	111	GLU
1	B	129	ASP
1	C	14	SER
1	C	16	ARG
1	C	28	GLU
1	C	31	SER
1	C	53	LEU
1	C	68	ASP
1	C	80	ASN
1	C	102	ASP
1	C	108	GLU
1	C	129	ASP
1	D	14	SER
1	D	28	GLU
1	D	31	SER
1	D	34	LYS
1	D	53	LEU
1	D	102	ASP
1	D	107	LYS

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Mol	Chain	Res	Type
1	D	129	ASP
1	D	150	PRO
1	E	14	SER
1	E	31	SER
1	E	53	LEU
1	E	80	ASN
1	F	14	SER
1	F	28	GLU
1	F	31	SER
1	F	53	LEU
1	F	80	ASN
1	F	102	ASP
1	F	107	LYS
1	F	108	GLU
1	F	129	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	88	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	EPE	B	165	-	15,15,15	0.84	1 (6%)	18,20,20	1.71	4 (22%)
2	EPE	D	165	-	15,15,15	0.86	1 (6%)	18,20,20	1.97	6 (33%)
3	SO3	B	168	-	1,3,3	0.40	0	0,3,3	0.00	-
3	SO3	F	165	-	1,3,3	0.55	0	0,3,3	0.00	-
2	EPE	B	166	-	15,15,15	0.75	1 (6%)	18,20,20	1.84	3 (16%)
2	EPE	C	165	-	15,15,15	0.89	1 (6%)	18,20,20	1.79	5 (27%)
2	EPE	A	165	-	15,15,15	0.95	1 (6%)	18,20,20	1.95	6 (33%)
3	SO3	B	167	-	1,3,3	0.52	0	0,3,3	0.00	-

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	EPE	B	165	-	-	4/9/19/19	0/1/1/1
2	EPE	C	165	-	-	4/9/19/19	0/1/1/1
2	EPE	A	165	-	-	4/9/19/19	0/1/1/1
2	EPE	B	166	-	-	7/9/19/19	0/1/1/1
2	EPE	D	165	-	-	1/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	165	EPE	C10-S	3.18	1.82	1.77
2	C	165	EPE	C10-S	3.07	1.81	1.77
2	D	165	EPE	C10-S	2.78	1.81	1.77
2	B	165	EPE	C10-S	2.44	1.81	1.77
2	B	166	EPE	C10-S	2.39	1.80	1.77

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	166	EPE	C5-N4-C3	4.62	119.24	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	165	EPE	O1S-S-C10	4.59	112.44	106.92
2	A	165	EPE	C5-N4-C3	4.43	118.79	108.83
2	B	165	EPE	C5-N4-C3	4.08	118.00	108.83
2	C	165	EPE	C5-N4-C3	3.88	117.57	108.83
2	D	165	EPE	C5-N4-C3	3.60	116.94	108.83
2	A	165	EPE	C7-N4-C5	3.57	120.35	111.23
2	B	165	EPE	O3S-S-C10	3.53	111.47	105.77
2	B	166	EPE	C7-N4-C5	3.51	120.20	111.23
2	B	166	EPE	C7-N4-C3	3.46	120.08	111.23
2	A	165	EPE	C7-N4-C3	3.45	120.06	111.23
2	C	165	EPE	O3S-S-C10	3.38	111.24	105.77
2	D	165	EPE	C7-N4-C3	3.35	119.81	111.23
2	C	165	EPE	C7-N4-C3	3.13	119.24	111.23
2	A	165	EPE	O3S-S-C10	2.74	110.21	105.77
2	D	165	EPE	C7-N4-C5	2.72	118.19	111.23
2	C	165	EPE	O2S-S-C10	2.67	110.13	106.92
2	B	165	EPE	C7-N4-C3	2.61	117.90	111.23
2	C	165	EPE	C7-N4-C5	2.56	117.77	111.23
2	A	165	EPE	O2S-S-C10	2.25	109.63	106.92
2	A	165	EPE	C6-N1-C2	2.17	113.72	108.83
2	D	165	EPE	C6-N1-C2	2.11	113.58	108.83
2	D	165	EPE	O2S-S-C10	2.07	109.41	106.92
2	B	165	EPE	C9-N1-C6	-2.04	106.02	111.23

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	165	EPE	C8-C7-N4-C3
2	B	166	EPE	C10-C9-N1-C2
2	B	166	EPE	C8-C7-N4-C5
2	B	166	EPE	S-C10-C9-N1
2	B	166	EPE	C9-C10-S-O1S
2	B	166	EPE	C9-C10-S-O3S
2	C	165	EPE	C8-C7-N4-C3
2	C	165	EPE	C9-C10-S-O1S
2	A	165	EPE	C10-C9-N1-C6
2	A	165	EPE	C9-C10-S-O3S
2	B	165	EPE	N4-C7-C8-O8
2	C	165	EPE	C9-C10-S-O3S
2	B	165	EPE	S-C10-C9-N1
2	B	165	EPE	C8-C7-N4-C5

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Mol	Chain	Res	Type	Atoms
2	B	166	EPE	C9-C10-S-O2S
2	C	165	EPE	C9-C10-S-O2S
2	A	165	EPE	C9-C10-S-O1S
2	A	165	EPE	C9-C10-S-O2S
2	B	165	EPE	C8-C7-N4-C3
2	B	166	EPE	C10-C9-N1-C6

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	165	EPE	5	0
2	B	166	EPE	2	0
2	C	165	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	152/164 (92%)	-0.25	1 (0%) 87 86	42, 59, 81, 104	0
1	B	152/164 (92%)	-0.31	0 100 100	38, 57, 81, 95	2 (1%)
1	C	151/164 (92%)	-0.29	0 100 100	41, 57, 79, 93	1 (0%)
1	D	150/164 (91%)	-0.30	0 100 100	42, 58, 78, 93	1 (0%)
1	E	133/164 (81%)	0.03	7 (5%) 26 20	43, 59, 82, 120	0
1	F	143/164 (87%)	-0.20	0 100 100	41, 59, 77, 97	1 (0%)
All	All	881/984 (89%)	-0.23	8 (0%) 84 83	38, 59, 81, 120	5 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	31	SER	3.4
1	E	109	PRO	2.9
1	E	13	LEU	2.8
1	E	141	MET	2.7
1	E	68	ASP	2.4
1	E	92	PHE	2.4
1	A	55	ILE	2.2
1	E	140	TYR	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, 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
3	SO3	F	165	4/4	0.82	0.19	38,55,59,61	1
3	SO3	B	167	4/4	0.88	0.17	60,62,75,78	1
2	EPE	C	165	15/15	0.90	0.29	46,54,74,80	9
2	EPE	B	166	15/15	0.93	0.23	46,58,75,76	7
2	EPE	A	165	15/15	0.94	0.16	66,72,80,86	2
2	EPE	D	165	15/15	0.95	0.15	49,67,75,82	2
2	EPE	B	165	15/15	0.96	0.20	37,56,62,62	7
3	SO3	B	168	4/4	0.97	0.16	49,55,66,69	1

6.5 Other polymers [i](#)

There are no such residues in this entry.