



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:45 PM UTC

PDB ID : 5W1U / pdb_00005w1u
Title : Culex quinquefasciatus carboxylesterase B2
Authors : Hopkins, D.H.; Jackson, C.J.
Deposited on : 2017-06-04
Resolution : 2.50 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

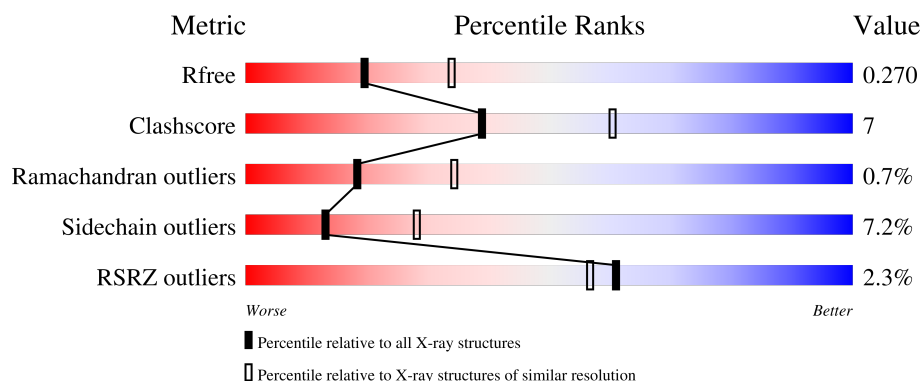
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	540	2% 81% 17% ..
1	B	540	3% 78% 20% ..

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
3	MLI	B	601	-	X	X	-

2 Entry composition [i](#)

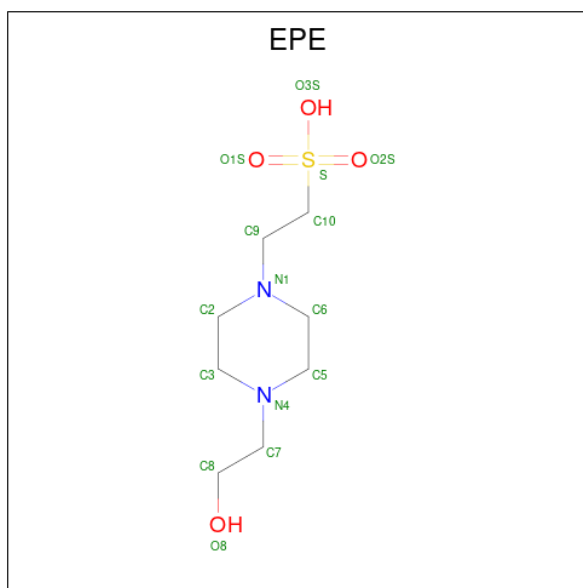
There are 4 unique types of molecules in this entry. The entry contains 17173 atoms, of which 8380 are hydrogens and 0 are deuteriums.

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 Carboxylic ester hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	536	Total	C	H	N	O	S	0	0	0
			8409	2705	4169	722	788	25			
1	B	537	Total	C	H	N	O	S	0	0	0
			8422	2710	4173	723	791	25			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			32	8	17	2	4	1		

- Molecule 3 is MALONATE ION (CCD ID: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			9	3	2	4		
3	B	1	Total	C	H	O	0	0
			9	3	2	4		

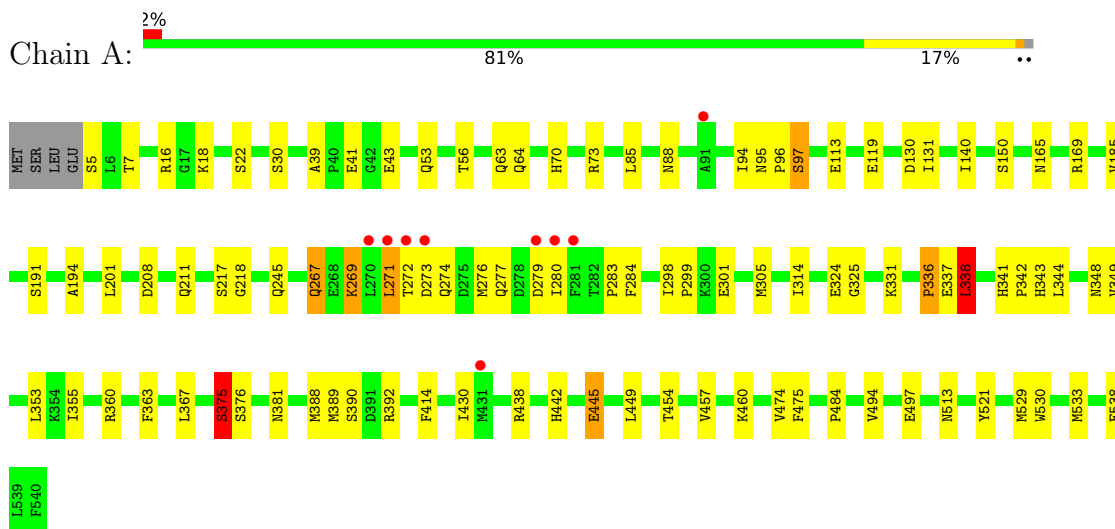
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	135	Total	O	0	0
			135	135		

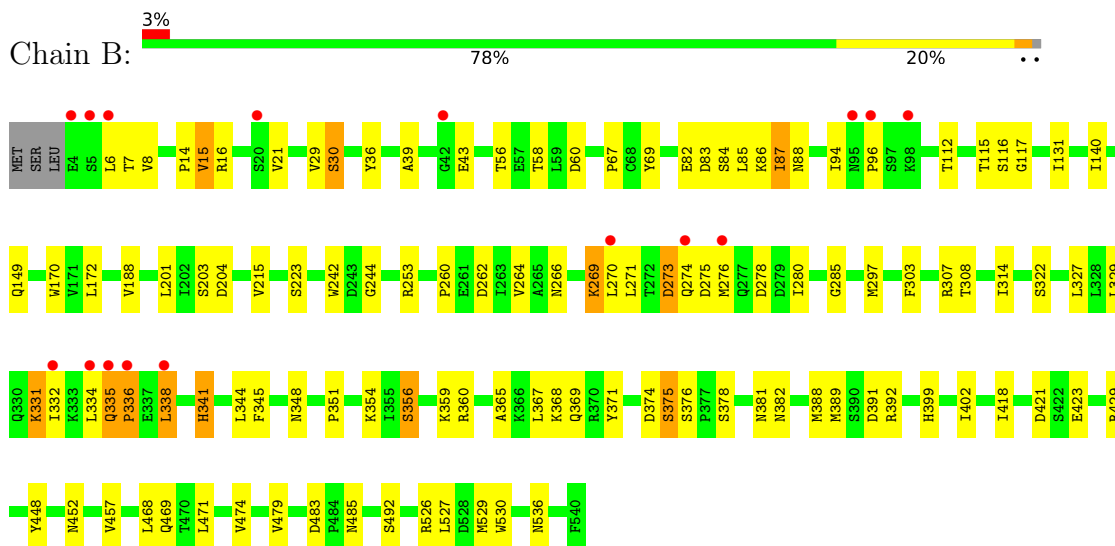
3 Residue-property plots [i](#)

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: Carboxylic ester hydrolase



• Molecule 1: Carboxylic ester hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.07Å 125.07Å 168.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.58 – 2.50 45.58 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.58-2.50) 99.9 (45.58-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.195 , 0.270 0.198 , 0.270	Depositor DCC
R_{free} test set	2599 reflections (3.83%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17173	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: EPE, MLI

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	0.97	1/4345 (0.0%)	1.10	13/5888 (0.2%)
1	B	0.94	3/4354 (0.1%)	1.07	9/5900 (0.2%)
All	All	0.95	4/8699 (0.0%)	1.09	22/11788 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	402	ILE	CA-CB	5.93	1.62	1.54
1	B	215	VAL	CA-CB	-5.50	1.47	1.54
1	B	188	VAL	CA-CB	-5.13	1.48	1.54
1	A	85	LEU	CA-C	-5.11	1.47	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	GLU	CA-C-N	7.79	127.35	119.24
1	A	301	GLU	C-N-CA	7.79	127.35	119.24
1	A	349	VAL	N-CA-C	-7.61	102.09	108.63
1	A	298	ILE	CA-C-N	6.76	126.22	118.85
1	A	298	ILE	C-N-CA	6.76	126.22	118.85
1	B	376	SER	CA-C-N	-6.49	113.30	119.85
1	B	376	SER	C-N-CA	-6.49	113.30	119.85
1	A	457	VAL	CA-C-N	-6.46	113.33	119.85
1	A	457	VAL	C-N-CA	-6.46	113.33	119.85
1	A	445	GLU	N-CA-C	-6.15	105.74	113.18
1	A	338	LEU	N-CA-C	-5.76	106.10	113.01
1	A	497	GLU	CA-C-N	-5.69	114.10	119.85
1	A	497	GLU	C-N-CA	-5.69	114.10	119.85
1	B	36	TYR	N-CA-C	-5.65	107.02	114.31
1	B	285	GLY	CA-C-N	5.61	125.63	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	GLY	C-N-CA	5.61	125.63	119.90
1	A	375	SER	N-CA-C	-5.61	98.86	110.80
1	B	457	VAL	CA-C-N	-5.45	114.09	119.92
1	B	457	VAL	C-N-CA	-5.45	114.09	119.92
1	B	418	ILE	N-CA-C	5.32	115.43	107.51
1	B	131	ILE	N-CA-C	5.12	114.78	108.53
1	A	442	HIS	N-CA-C	-5.00	102.51	109.96

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4240	4169	4166	48	0
1	B	4249	4173	4172	66	0
2	A	15	17	17	0	0
2	B	15	17	17	0	0
3	A	7	2	2	1	0
3	B	7	2	2	2	0
4	A	125	0	0	10	0
4	B	135	0	0	7	0
All	All	8793	8380	8376	115	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 7.

All (115) 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:B:307:ARG:NH2	4:B:701:HOH:O	2.12	0.81
1:A:454:THR:O	4:A:701:HOH:O	2.06	0.73
1:A:513:ASN:O	4:A:702:HOH:O	2.12	0.67
1:A:267:GLN:O	1:A:271:LEU:HD22	1.96	0.66
1:B:479:VAL:O	4:B:703:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLU:OE1	4:B:702:HOH:O	2.13	0.65
1:A:445:GLU:OE2	4:A:703:HOH:O	2.16	0.63
1:A:460:LYS:N	4:A:715:HOH:O	2.32	0.62
1:A:521:TYR:O	4:A:704:HOH:O	2.16	0.61
1:B:327:LEU:HD21	3:B:601:MLI:H12	1.81	0.61
1:A:360:ARG:NH1	4:A:707:HOH:O	2.21	0.58
1:B:276:MET:HA	1:B:280:ILE:HG22	1.85	0.58
1:B:273:ASP:N	1:B:273:ASP:OD1	2.35	0.58
1:A:39:ALA:O	1:A:41:GLU:N	2.36	0.58
1:B:327:LEU:CD2	3:B:601:MLI:H12	2.34	0.58
1:B:391:ASP:OD2	1:B:526:ARG:HD2	2.04	0.58
1:B:483:ASP:OD1	1:B:485:ASN:ND2	2.37	0.57
1:B:348:ASN:CG	1:B:389:MET:HE1	2.29	0.57
1:B:8:VAL:N	1:B:15:VAL:O	2.30	0.57
1:A:165:ASN:OD1	1:A:169:ARG:NE	2.36	0.57
1:A:343:HIS:ND1	4:A:714:HOH:O	2.31	0.57
1:A:342:PRO:O	4:A:705:HOH:O	2.17	0.56
1:B:262:ASP:O	1:B:266:ASN:ND2	2.34	0.56
1:A:271:LEU:HD23	1:A:283:PRO:CG	2.35	0.56
1:B:115:THR:HG22	1:B:117:GLY:H	1.71	0.56
1:B:375:SER:HB2	1:B:381:ASN:ND2	2.21	0.56
1:A:363:PHE:HB3	1:A:533:MET:HE2	1.88	0.55
1:B:421:ASP:OD1	1:B:429:ARG:NH1	2.40	0.55
1:A:271:LEU:HD21	1:A:284:PHE:CE2	2.43	0.54
1:B:360:ARG:HD3	4:B:777:HOH:O	2.08	0.54
1:A:367:LEU:HD21	1:A:533:MET:HE1	1.90	0.54
1:B:367:LEU:HB3	1:B:388:MET:CE	2.37	0.54
1:B:8:VAL:O	1:B:15:VAL:N	2.39	0.54
1:A:325:GLY:N	1:A:390:SER:OG	2.36	0.53
1:A:336:PRO:C	1:A:338:LEU:H	2.17	0.53
1:B:84:SER:O	1:B:86:LYS:N	2.40	0.53
1:A:271:LEU:CD2	1:A:283:PRO:CG	2.88	0.52
1:B:115:THR:HG22	1:B:116:SER:N	2.24	0.52
1:B:354:LYS:HE3	1:B:536:ASN:HB3	1.91	0.52
1:B:338:LEU:O	1:B:341:HIS:HB2	2.10	0.52
1:B:375:SER:HB2	1:B:381:ASN:HD21	1.75	0.52
1:B:67:PRO:HB3	1:B:115:THR:HG23	1.92	0.51
1:A:217:SER:OG	1:A:324:GLU:OE2	2.20	0.51
1:A:73:ARG:NE	1:A:113:GLU:OE1	2.44	0.51
1:B:201:LEU:CD2	1:B:314:ILE:HD11	2.41	0.50
1:B:448:TYR:HB2	1:B:471:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:HG22	1:A:96:PRO:HD3	1.94	0.50
3:A:601:MLI:O8	4:A:706:HOH:O	2.18	0.50
1:B:203:SER:OG	1:B:297:MET:O	2.24	0.50
1:A:267:GLN:C	1:A:271:LEU:HD22	2.37	0.49
1:A:94:ILE:HD12	1:A:94:ILE:N	2.28	0.49
1:A:271:LEU:CD2	1:A:283:PRO:HG2	2.42	0.49
1:B:201:LEU:HD21	1:B:314:ILE:HD11	1.93	0.49
1:B:351:PRO:HA	1:B:360:ARG:HH12	1.77	0.49
1:A:194:ALA:HB3	1:A:218:GLY:HA3	1.95	0.48
1:B:16:ARG:NH2	1:B:60:ASP:OD1	2.47	0.48
1:A:185:VAL:N	1:A:211:GLN:OE1	2.45	0.48
1:A:388:MET:HG2	1:A:389:MET:HE2	1.97	0.47
1:B:345:PHE:CE1	1:B:368:LYS:HA	2.50	0.47
1:B:356:SER:OG	4:B:704:HOH:O	2.17	0.47
1:A:276:MET:HB3	1:A:280:ILE:HG22	1.97	0.46
1:A:299:PRO:HD2	1:A:305:MET:SD	2.55	0.46
1:A:7:THR:HG22	1:A:16:ARG:HB2	1.97	0.46
1:B:94:ILE:N	1:B:94:ILE:HD12	2.30	0.46
1:A:348:ASN:CG	1:A:389:MET:HE1	2.41	0.46
1:B:94:ILE:HG22	1:B:96:PRO:HD3	1.98	0.46
1:A:375:SER:OG	1:A:381:ASN:OD1	2.30	0.45
1:B:29:VAL:HG11	1:B:94:ILE:HD11	1.98	0.45
1:B:242:TRP:CZ3	1:B:244:GLY:HA2	2.52	0.45
1:B:266:ASN:HA	1:B:269:LYS:HB2	1.99	0.45
1:A:341:HIS:CE1	1:A:343:HIS:HB2	2.53	0.44
1:A:392:ARG:HG3	1:A:530:TRP:CH2	2.52	0.44
1:B:367:LEU:HB3	1:B:388:MET:HE1	1.99	0.44
1:A:95:ASN:C	1:A:97:SER:H	2.26	0.44
1:B:29:VAL:HG12	1:B:30:SER:N	2.33	0.44
1:B:367:LEU:HD23	1:B:529:MET:HE3	1.98	0.44
1:B:280:ILE:HG23	1:B:280:ILE:O	2.18	0.44
1:B:371:TYR:CD2	1:B:388:MET:HE3	2.52	0.44
1:A:325:GLY:H	1:A:390:SER:HG	1.59	0.43
1:B:115:THR:HG22	1:B:116:SER:H	1.83	0.43
1:A:88:ASN:ND2	4:A:730:HOH:O	2.52	0.43
1:A:474:VAL:HG23	1:A:475:PHE:N	2.32	0.43
1:B:354:LYS:O	1:B:354:LYS:HG3	2.19	0.43
1:B:14:PRO:HB2	1:B:58:THR:HA	2.01	0.43
1:B:354:LYS:HE2	4:B:791:HOH:O	2.18	0.43
1:A:64:GLN:NE2	1:A:119:GLU:OE1	2.45	0.42
1:B:39:ALA:HB2	1:B:83:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASN:O	1:B:271:LEU:HD23	2.18	0.42
1:A:191:SER:HA	1:A:217:SER:O	2.20	0.42
1:B:367:LEU:HD23	1:B:529:MET:CE	2.48	0.42
1:B:335:GLN:N	1:B:336:PRO:HD3	2.34	0.42
1:A:70:HIS:CD2	1:A:113:GLU:HB2	2.55	0.42
1:A:529:MET:HE2	1:A:529:MET:HB3	1.89	0.42
1:B:365:ALA:O	1:B:369:GLN:HG2	2.20	0.42
1:B:399:HIS:HB2	1:B:527:LEU:HD13	2.01	0.42
1:A:348:ASN:OD1	1:A:389:MET:HE1	2.19	0.42
1:B:87:ILE:HD13	1:B:170:TRP:CZ3	2.55	0.42
1:B:39:ALA:HB2	1:B:83:ASP:CG	2.45	0.42
1:B:87:ILE:HD13	1:B:170:TRP:CE3	2.54	0.42
1:B:389:MET:HA	1:B:389:MET:HE2	2.01	0.41
1:B:276:MET:C	1:B:278:ASP:N	2.77	0.41
1:A:414:PHE:CD1	1:A:484:PRO:HG3	2.56	0.41
1:A:201:LEU:HD21	1:A:314:ILE:HD11	2.03	0.41
1:B:332:ILE:HD12	1:B:338:LEU:HB3	2.03	0.41
1:A:274:GLN:C	1:A:276:MET:H	2.28	0.41
1:B:331:LYS:O	1:B:334:LEU:N	2.48	0.41
1:B:69:TYR:CE1	1:B:260:PRO:HB2	2.56	0.41
1:B:303:PHE:HB2	4:B:744:HOH:O	2.21	0.41
1:B:468:LEU:HD23	1:B:468:LEU:C	2.46	0.41
1:A:271:LEU:HG	1:A:283:PRO:HG3	2.04	0.40
1:B:329:LEU:HD11	1:B:382:ASN:HD22	1.85	0.40
1:B:526:ARG:O	1:B:529:MET:HB3	2.21	0.40
1:B:392:ARG:HG3	1:B:530:TRP:CH2	2.57	0.40
1:A:353:LEU:HB2	1:A:355:ILE:HG12	2.02	0.40
1:B:274:GLN:O	1:B:275:ASP:HB2	2.22	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	534/540 (99%)	479 (90%)	50 (9%)	5 (1%)	14	27
1	B	535/540 (99%)	487 (91%)	45 (8%)	3 (1%)	21	38
All	All	1069/1080 (99%)	966 (90%)	95 (9%)	8 (1%)	18	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	A	269	LYS
1	A	208	ASP
1	A	279	ASP
1	A	336	PRO
1	B	85	LEU
1	B	336	PRO
1	B	264	VAL

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	457/461 (99%)	427 (93%)	30 (7%)	15	32
1	B	458/461 (99%)	422 (92%)	36 (8%)	11	24
All	All	915/922 (99%)	849 (93%)	66 (7%)	13	28

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	18	LYS
1	A	22	SER
1	A	30	SER
1	A	43	GLU
1	A	53	GLN
1	A	56	THR
1	A	63	GLN

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Mol	Chain	Res	Type
1	A	97	SER
1	A	130	ASP
1	A	131	ILE
1	A	140	ILE
1	A	150	SER
1	A	245	GLN
1	A	269	LYS
1	A	271	LEU
1	A	272	THR
1	A	273	ASP
1	A	277	GLN
1	A	331	LYS
1	A	337	GLU
1	A	338	LEU
1	A	344	LEU
1	A	375	SER
1	A	376	SER
1	A	430	ILE
1	A	438	ARG
1	A	449	LEU
1	A	494	VAL
1	A	538	GLU
1	B	6	LEU
1	B	7	THR
1	B	15	VAL
1	B	21	VAL
1	B	30	SER
1	B	43	GLU
1	B	56	THR
1	B	87	ILE
1	B	88	ASN
1	B	112	THR
1	B	140	ILE
1	B	149	GLN
1	B	172	LEU
1	B	204	ASP
1	B	223	SER
1	B	253	ARG
1	B	269	LYS
1	B	270	LEU
1	B	273	ASP
1	B	308	THR

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Mol	Chain	Res	Type
1	B	322	SER
1	B	331	LYS
1	B	335	GLN
1	B	338	LEU
1	B	341	HIS
1	B	344	LEU
1	B	356	SER
1	B	359	LYS
1	B	374	ASP
1	B	375	SER
1	B	378	SER
1	B	423	GLU
1	B	452	ASN
1	B	469	GLN
1	B	474	VAL
1	B	492	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	231	ASN
1	A	274	GLN
1	A	499	ASN
1	B	95	ASN
1	B	231	ASN
1	B	245	GLN
1	B	267	GLN
1	B	274	GLN
1	B	387	HIS
1	B	456	GLN
1	B	536	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	MLI	B	601	-	6,6,6	0.91	0	7,7,7	2.09	3 (42%)
2	EPE	B	600	-	15,15,15	1.96	2 (13%)	19,20,20	2.53	10 (52%)
2	EPE	A	600	-	15,15,15	1.42	1 (6%)	19,20,20	2.01	5 (26%)
3	MLI	A	601	-	6,6,6	1.07	0	7,7,7	1.82	2 (28%)

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	MLI	B	601	-	-	4/4/4/4	-
2	EPE	B	600	-	-	3/9/19/19	0/1/1/1
2	EPE	A	600	-	-	1/9/19/19	0/1/1/1
3	MLI	A	601	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	EPE	C10-S	6.38	1.86	1.77
2	A	600	EPE	C10-S	4.86	1.84	1.77
2	B	600	EPE	C9-N1	2.53	1.53	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	EPE	O2S-S-C10	5.28	114.71	106.73
2	B	600	EPE	O2S-S-C10	5.25	114.67	106.73
2	B	600	EPE	C3-C2-N1	4.79	120.32	110.65
2	B	600	EPE	C7-N4-C5	3.54	120.68	111.24
2	A	600	EPE	C7-N4-C5	3.31	120.07	111.24
2	B	600	EPE	C2-C3-N4	3.25	117.21	110.65
3	B	601	MLI	C3-C1-C2	-3.20	101.66	112.95
2	A	600	EPE	C7-N4-C3	3.18	119.70	111.24
3	B	601	MLI	O8-C3-C1	-3.14	113.17	122.11
2	B	600	EPE	O2S-S-O1S	-3.05	103.90	113.82
3	A	601	MLI	C3-C1-C2	-2.71	103.38	112.95
3	A	601	MLI	O9-C3-C1	2.65	122.73	114.51
2	B	600	EPE	O3S-S-O1S	-2.64	104.81	111.40
3	B	601	MLI	O9-C3-C1	2.60	122.57	114.51
2	A	600	EPE	O3S-S-O1S	-2.55	105.01	111.40
2	B	600	EPE	C5-N4-C3	2.50	114.23	108.84
2	A	600	EPE	C9-N1-C6	2.37	117.55	111.24
2	B	600	EPE	O3S-S-C10	2.35	110.59	106.00
2	B	600	EPE	C7-N4-C3	2.30	117.36	111.24
2	B	600	EPE	O1S-S-C10	2.25	110.13	106.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	EPE	C10-C9-N1-C6
2	A	600	EPE	C9-C10-S-O3S
2	B	600	EPE	C10-C9-N1-C2
2	B	600	EPE	C9-C10-S-O3S
3	A	601	MLI	C2-C1-C3-O8
3	A	601	MLI	C2-C1-C3-O9
3	B	601	MLI	C2-C1-C3-O9
3	B	601	MLI	C2-C1-C3-O8
3	B	601	MLI	C3-C1-C2-O6
3	B	601	MLI	C3-C1-C2-O7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	MLI	2	0
3	A	601	MLI	1	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	536/540 (99%)	-0.12	9 (1%) 69 65	22, 51, 86, 139	0
1	B	537/540 (99%)	0.01	16 (2%) 52 48	22, 53, 95, 264	0
All	All	1073/1080 (99%)	-0.05	25 (2%) 61 57	22, 52, 92, 264	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	LEU	5.4
1	A	270	LEU	4.7
1	A	271	LEU	4.6
1	B	332	ILE	4.6
1	B	4	GLU	4.0
1	A	272	THR	3.6
1	A	273	ASP	3.4
1	B	270	LEU	3.4
1	B	5	SER	3.3
1	B	335	GLN	3.3
1	B	338	LEU	3.2
1	B	96	PRO	2.6
1	A	279	ASP	2.6
1	A	91	ALA	2.5
1	A	431	MET	2.5
1	B	6	LEU	2.4
1	A	281	PHE	2.4
1	B	98	LYS	2.3
1	B	20	SER	2.3
1	B	336	PRO	2.3
1	B	95	ASN	2.1
1	B	274	GLN	2.1
1	B	42	GLY	2.1
1	B	276	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	280	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EPE	B	600	15/15	0.87	0.16	47,61,83,101	0
2	EPE	A	600	15/15	0.90	0.13	42,60,79,91	0
3	MLI	A	601	7/7	0.91	0.16	53,76,93,93	0
3	MLI	B	601	7/7	0.92	0.17	38,60,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.