wwPDB EM Map/Model Validation Report (i)

Jun 13, 2016 – 03:05 PM EDT

PDB ID	:	5IS0
EMDB ID:	:	EMD-8119
Title	:	Structure of TRPV1 in complex with capsazepine, determined in lipid nanodisc
Authors	:	Gao, Y.; Cao, E.; Julius, D.; Cheng, Y.
Deposited on	:	2016-03-15
Resolution	:	3.43 Å(reported)
Based on PDB ID	:	3J5P

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

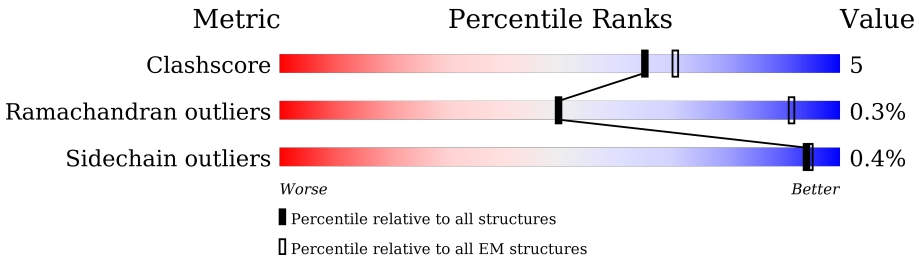
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.43 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	B	636	54% 8% 38%
1	C	636	54% 7% 38%
1	D	636	54% 7% 38%
1	E	636	54% 8% 38%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11892 atoms, of which 84 are hydrogens and 0 are deuteriums.

In the tables below, 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.

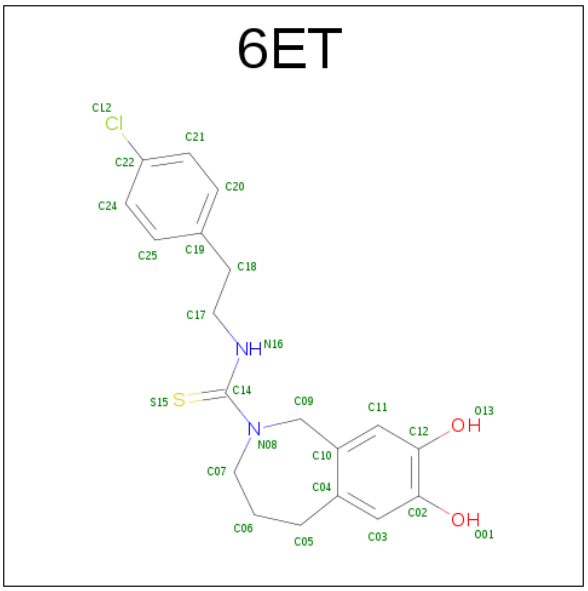
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily V member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	394	Total	C	N	O	S	0	0
			2927	1932	481	496	18		
1	B	394	Total	C	N	O	S	0	0
			2927	1932	481	496	18		
1	D	394	Total	C	N	O	S	0	0
			2927	1932	481	496	18		
1	E	394	Total	C	N	O	S	0	0
			2927	1932	481	496	18		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	106	ALA	-	expression tag	UNP O35433
C	107	MET	-	expression tag	UNP O35433
C	108	GLY	-	expression tag	UNP O35433
C	109	SER	-	expression tag	UNP O35433
B	106	ALA	-	expression tag	UNP O35433
B	107	MET	-	expression tag	UNP O35433
B	108	GLY	-	expression tag	UNP O35433
B	109	SER	-	expression tag	UNP O35433
D	106	ALA	-	expression tag	UNP O35433
D	107	MET	-	expression tag	UNP O35433
D	108	GLY	-	expression tag	UNP O35433
D	109	SER	-	expression tag	UNP O35433
E	106	ALA	-	expression tag	UNP O35433
E	107	MET	-	expression tag	UNP O35433
E	108	GLY	-	expression tag	UNP O35433
E	109	SER	-	expression tag	UNP O35433

- Molecule 2 is capsazepine (three-letter code: 6ET) (formula: $C_{19}H_{21}ClN_2O_2S$).



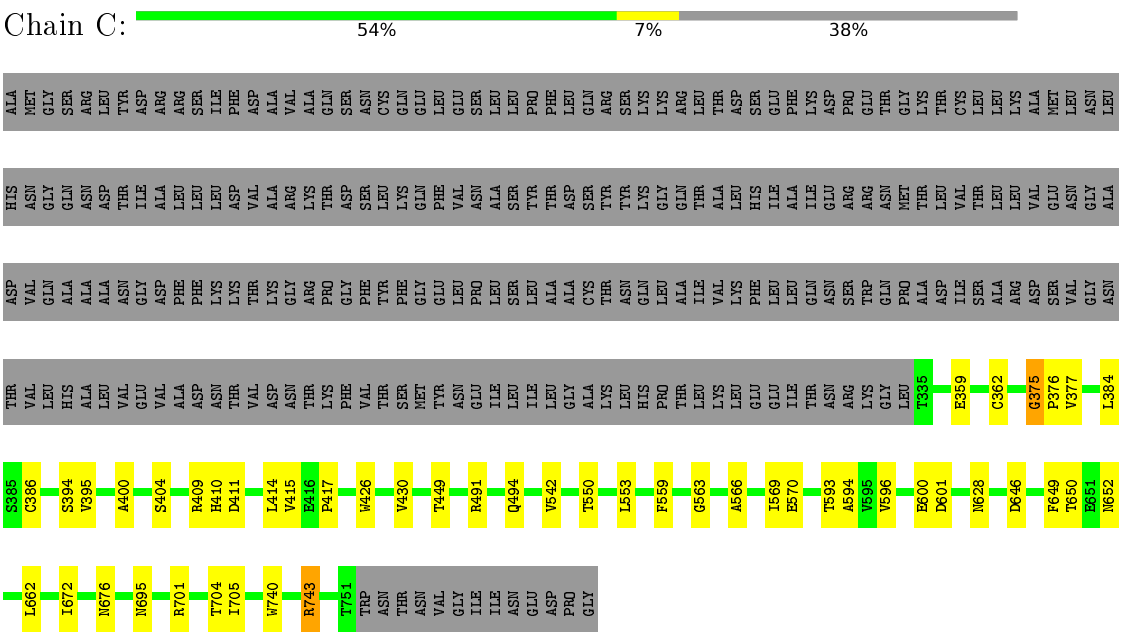
Mol	Chain	Residues	Atoms							AltConf
2	C	1	Total	C	Cl	H	N	O	S	0
			46	19	1	21	2	2	1	
2	B	1	Total	C	Cl	H	N	O	S	0
			46	19	1	21	2	2	1	
2	D	1	Total	C	Cl	H	N	O	S	0
			46	19	1	21	2	2	1	
2	E	1	Total	C	Cl	H	N	O	S	0
			46	19	1	21	2	2	1	

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

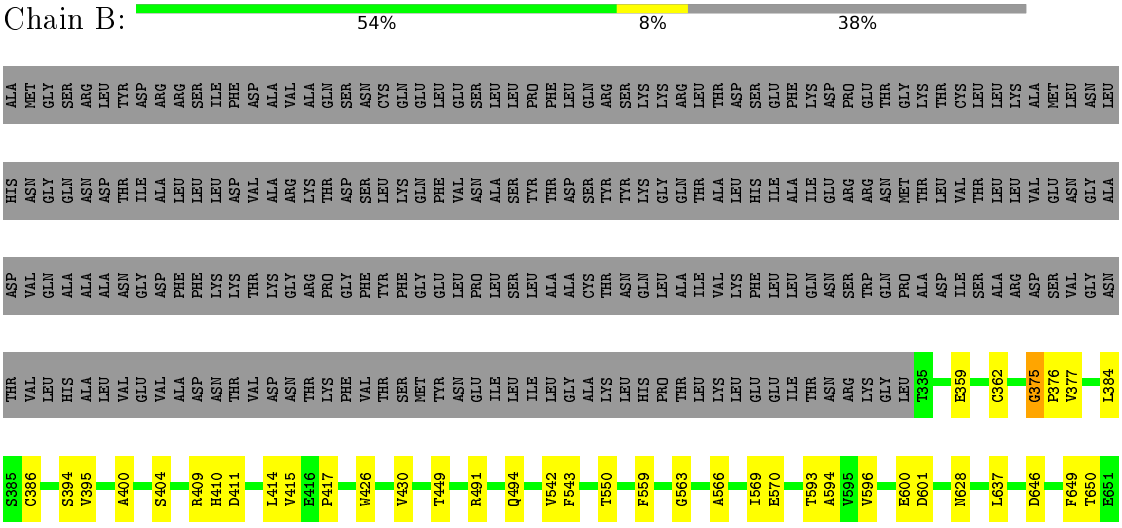
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain C:



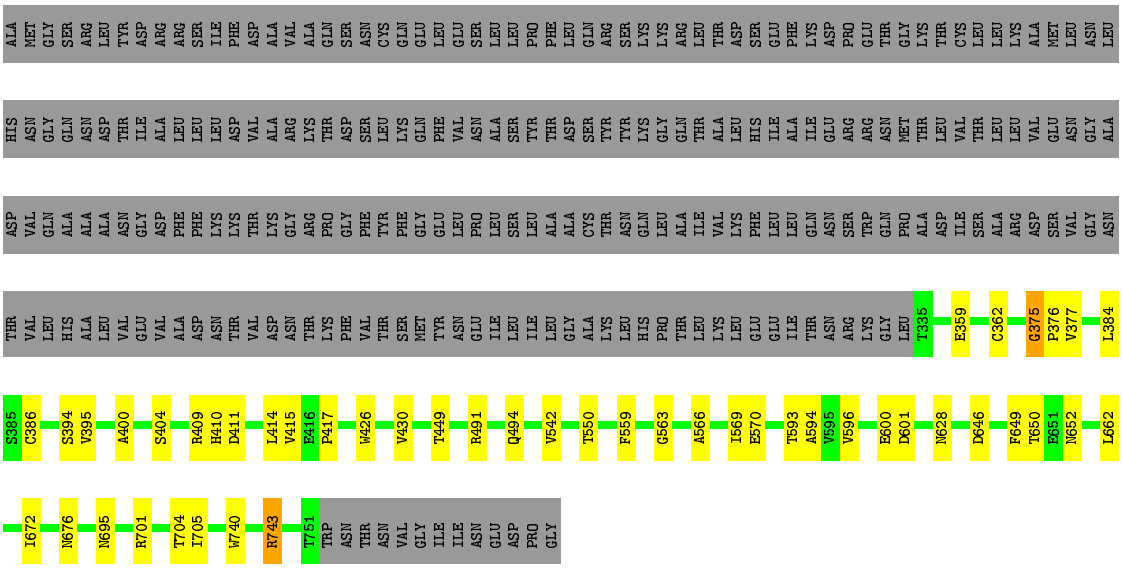
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain B:



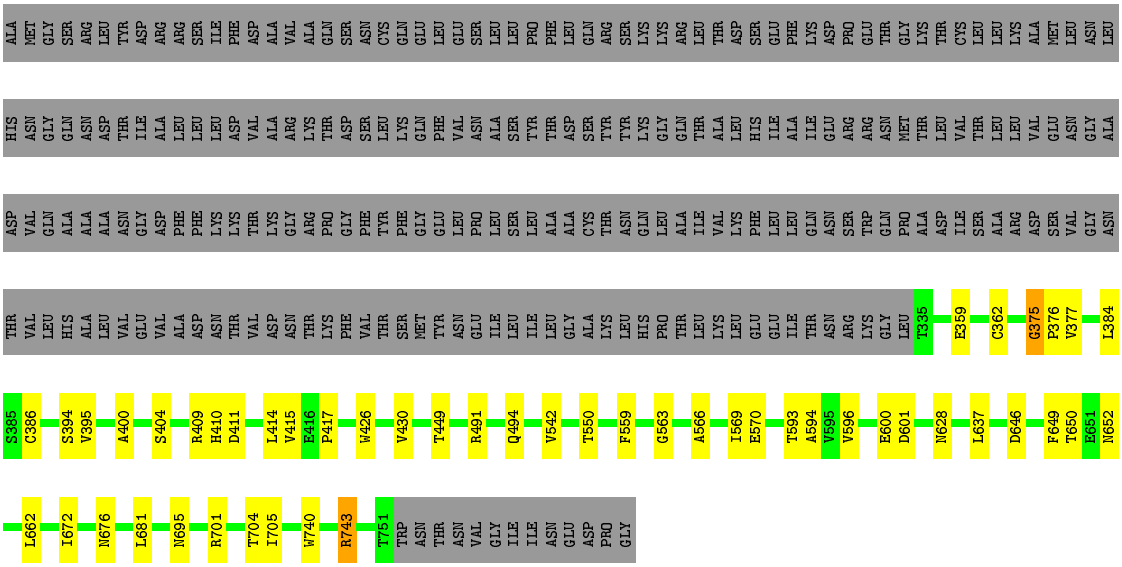
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain D:



• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain E:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	80725	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	31000	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6ET

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	B	0.69	1/2992 (0.0%)	0.63	1/4064 (0.0%)
1	C	0.69	1/2992 (0.0%)	0.63	1/4064 (0.0%)
1	D	0.69	1/2992 (0.0%)	0.63	1/4064 (0.0%)
1	E	0.69	1/2992 (0.0%)	0.63	1/4064 (0.0%)
All	All	0.69	4/11968 (0.0%)	0.63	4/16256 (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	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	596	VAL	CB-CG2	-5.84	1.40	1.52
1	C	596	VAL	CB-CG2	-5.83	1.40	1.52
1	D	596	VAL	CB-CG2	-5.83	1.40	1.52
1	B	596	VAL	CB-CG2	-5.81	1.40	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	662	LEU	CB-CG-CD1	-5.34	101.92	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	662	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	D	662	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	C	662	LEU	CB-CG-CD1	-5.30	101.98	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	375	GLY	Peptide
1	B	740	TRP	Peptide
1	C	375	GLY	Peptide
1	C	740	TRP	Peptide
1	D	375	GLY	Peptide
1	D	740	TRP	Peptide
1	E	375	GLY	Peptide
1	E	740	TRP	Peptide

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	B	2927	0	2746	33	0
1	C	2927	0	2746	30	0
1	D	2927	0	2746	30	0
1	E	2927	0	2746	31	0
2	B	25	21	0	5	0
2	C	25	21	0	5	0
2	D	25	21	0	4	0
2	E	25	21	0	4	0
All	All	11808	84	10984	116	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 5.

All (116) 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:550:THR:OG1	2:C:801:6ET:S15	2.16	1.01
1:D:550:THR:OG1	2:D:801:6ET:S15	2.19	0.99
1:E:550:THR:OG1	2:E:801:6ET:S15	2.21	0.98
1:B:550:THR:OG1	2:B:801:6ET:S15	2.21	0.97
1:C:550:THR:CB	2:C:801:6ET:S15	2.70	0.80
1:D:550:THR:CB	2:D:801:6ET:S15	2.71	0.78
1:E:550:THR:CB	2:E:801:6ET:S15	2.73	0.76
1:B:550:THR:CB	2:B:801:6ET:S15	2.75	0.74
1:C:550:THR:HB	2:C:801:6ET:S15	2.38	0.64
1:B:426:TRP:HA	1:B:430:VAL:HG12	1.81	0.63
1:C:426:TRP:HA	1:C:430:VAL:HG12	1.80	0.63
1:E:426:TRP:HA	1:E:430:VAL:HG12	1.80	0.63
1:D:426:TRP:HA	1:D:430:VAL:HG12	1.81	0.63
1:D:550:THR:HB	2:D:801:6ET:S15	2.38	0.62
1:E:550:THR:HB	2:E:801:6ET:S15	2.41	0.61
1:D:410:HIS:HB3	1:D:695:ASN:HB3	1.82	0.61
1:B:410:HIS:HB3	1:B:695:ASN:HB3	1.82	0.61
1:E:410:HIS:HB3	1:E:695:ASN:HB3	1.83	0.60
1:C:410:HIS:HB3	1:C:695:ASN:HB3	1.82	0.60
1:B:550:THR:HB	2:B:801:6ET:S15	2.43	0.58
1:D:411:ASP:HA	1:D:414:LEU:HD13	1.87	0.57
1:C:411:ASP:HA	1:C:414:LEU:HD13	1.87	0.57
1:E:411:ASP:HA	1:E:414:LEU:HD13	1.87	0.56
1:B:411:ASP:HA	1:B:414:LEU:HD13	1.87	0.56
1:B:400:ALA:O	1:B:409:ARG:NH2	2.39	0.56
1:E:400:ALA:O	1:E:409:ARG:NH2	2.39	0.56
1:D:400:ALA:O	1:D:409:ARG:NH2	2.39	0.55
1:C:400:ALA:O	1:C:409:ARG:NH2	2.39	0.55
1:C:594:ALA:HB1	1:D:542:VAL:HG13	1.89	0.53
1:B:542:VAL:HG13	1:E:594:ALA:HB1	1.91	0.53
1:C:542:VAL:HG13	1:B:594:ALA:HB1	1.92	0.52
1:E:570:GLU:OE2	2:E:801:6ET:O01	2.28	0.51
1:B:570:GLU:OE2	2:B:801:6ET:O01	2.29	0.51
1:D:600:GLU:O	1:D:628:ASN:ND2	2.44	0.51
1:B:600:GLU:O	1:B:628:ASN:ND2	2.44	0.50
1:E:600:GLU:O	1:E:628:ASN:ND2	2.44	0.50
1:D:650:THR:OG1	1:D:652:ASN:OD1	2.30	0.50
1:D:594:ALA:HB1	1:E:542:VAL:HG13	1.92	0.50
1:C:650:THR:OG1	1:C:652:ASN:OD1	2.30	0.50
1:E:650:THR:OG1	1:E:652:ASN:OD1	2.30	0.49
1:C:600:GLU:O	1:C:628:ASN:ND2	2.44	0.49
1:E:415:VAL:HG12	1:E:417:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:HG12	1:B:417:PRO:HD2	1.95	0.49
1:C:593:THR:HG21	1:D:449:THR:HG23	1.95	0.49
1:B:430:VAL:HG11	1:B:705:ILE:HG12	1.95	0.49
1:B:650:THR:OG1	1:B:652:ASN:OD1	2.30	0.49
1:D:430:VAL:HG11	1:D:705:ILE:HG12	1.95	0.48
1:D:570:GLU:OE2	2:D:801:6ET:O01	2.31	0.48
1:C:430:VAL:HG11	1:C:705:ILE:HG12	1.95	0.48
1:E:430:VAL:HG11	1:E:705:ILE:HG12	1.95	0.48
1:B:449:THR:HG23	1:E:593:THR:HG21	1.94	0.48
1:D:415:VAL:HG12	1:D:417:PRO:HD2	1.95	0.48
1:C:415:VAL:HG12	1:C:417:PRO:HD2	1.95	0.48
1:D:593:THR:HG21	1:E:449:THR:HG23	1.95	0.47
1:C:449:THR:HG23	1:B:593:THR:HG21	1.97	0.47
1:E:701:ARG:O	1:E:704:THR:OG1	2.29	0.47
1:B:386:CYS:O	1:B:394:SER:OG	2.34	0.46
1:D:601:ASP:O	1:D:652:ASN:ND2	2.49	0.46
1:B:601:ASP:O	1:B:652:ASN:ND2	2.49	0.46
1:D:386:CYS:O	1:D:394:SER:OG	2.34	0.45
1:D:559:PHE:O	1:D:563:GLY:N	2.48	0.45
1:C:570:GLU:OE2	2:C:801:6ET:O01	2.34	0.45
1:C:386:CYS:O	1:C:394:SER:OG	2.34	0.45
1:C:601:ASP:O	1:C:652:ASN:ND2	2.48	0.45
1:E:386:CYS:O	1:E:394:SER:OG	2.34	0.45
1:E:601:ASP:O	1:E:652:ASN:ND2	2.49	0.45
1:C:559:PHE:O	1:C:563:GLY:N	2.48	0.45
1:E:375:GLY:O	1:E:377:VAL:N	2.50	0.45
1:C:672:ILE:O	1:C:676:ASN:ND2	2.50	0.44
1:D:491:ARG:HA	1:D:494:GLN:HG2	1.99	0.44
1:D:672:ILE:O	1:D:676:ASN:ND2	2.50	0.44
1:C:375:GLY:O	1:C:377:VAL:N	2.50	0.44
1:C:701:ARG:O	1:C:704:THR:OG1	2.29	0.44
1:E:559:PHE:O	1:E:563:GLY:N	2.48	0.44
1:E:672:ILE:O	1:E:676:ASN:ND2	2.50	0.44
1:D:375:GLY:O	1:D:377:VAL:N	2.50	0.44
1:E:491:ARG:HA	1:E:494:GLN:HG2	1.99	0.44
1:B:375:GLY:O	1:B:377:VAL:N	2.50	0.44
1:B:384:LEU:HD22	1:B:743:ARG:HB2	2.00	0.44
1:B:708:THR:O	1:B:712:PHE:N	2.38	0.44
1:D:646:ASP:HB3	1:D:649:PHE:HB3	2.00	0.44
1:C:384:LEU:HD22	1:C:743:ARG:HB2	2.00	0.43
1:B:646:ASP:HB3	1:B:649:PHE:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:ARG:HA	1:C:494:GLN:HG2	1.99	0.43
1:C:646:ASP:HB3	1:C:649:PHE:HB3	2.00	0.43
1:B:672:ILE:O	1:B:676:ASN:ND2	2.50	0.43
1:B:701:ARG:O	1:B:704:THR:OG1	2.29	0.43
1:D:701:ARG:O	1:D:704:THR:OG1	2.29	0.43
1:E:384:LEU:HD22	1:E:743:ARG:HB2	2.00	0.43
1:E:566:ALA:HA	1:E:569:ILE:HD12	2.00	0.43
1:B:491:ARG:HA	1:B:494:GLN:HG2	1.99	0.43
1:C:566:ALA:HA	1:C:569:ILE:HD12	2.00	0.43
1:E:646:ASP:HB3	1:E:649:PHE:HB3	2.00	0.43
1:D:394:SER:OG	1:D:395:VAL:N	2.52	0.42
1:D:384:LEU:HD22	1:D:743:ARG:HB2	2.00	0.42
1:D:652:ASN:OD1	1:D:652:ASN:N	2.50	0.42
1:E:359:GLU:HB3	1:E:362:CYS:HB3	2.01	0.42
1:B:394:SER:OG	1:B:395:VAL:N	2.52	0.42
1:B:566:ALA:HA	1:B:569:ILE:HD12	2.00	0.42
1:C:359:GLU:HB3	1:C:362:CYS:HB3	2.01	0.42
1:D:566:ALA:HA	1:D:569:ILE:HD12	2.00	0.42
1:B:404:SER:HA	1:B:409:ARG:HD2	2.02	0.42
1:C:394:SER:OG	1:C:395:VAL:N	2.52	0.42
1:E:404:SER:HA	1:E:409:ARG:HD2	2.02	0.42
1:D:359:GLU:HB3	1:D:362:CYS:HB3	2.01	0.42
1:E:681:LEU:HA	1:E:681:LEU:HD23	1.89	0.42
1:B:652:ASN:OD1	1:B:652:ASN:N	2.50	0.41
1:B:359:GLU:HB3	1:B:362:CYS:HB3	2.01	0.41
1:E:394:SER:OG	1:E:395:VAL:N	2.52	0.41
1:D:404:SER:HA	1:D:409:ARG:HD2	2.02	0.41
1:B:559:PHE:O	1:B:563:GLY:N	2.48	0.41
1:C:404:SER:HA	1:C:409:ARG:HD2	2.02	0.41
1:B:543:PHE:CD1	2:B:801:6ET:CL2	3.11	0.41
1:C:553:LEU:HD12	2:C:801:6ET:C05	2.51	0.40
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.88	0.40
1:E:637:LEU:HA	1:E:637:LEU:HD23	1.87	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 PDB entries followed by that with respect to all EM entries.

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	B	392/636 (62%)	352 (90%)	39 (10%)	1 (0%)	46 83
1	C	392/636 (62%)	351 (90%)	40 (10%)	1 (0%)	46 83
1	D	392/636 (62%)	351 (90%)	40 (10%)	1 (0%)	46 83
1	E	392/636 (62%)	352 (90%)	39 (10%)	1 (0%)	46 83
All	All	1568/2544 (62%)	1406 (90%)	158 (10%)	4 (0%)	50 83

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	376	PRO
1	B	376	PRO
1	D	376	PRO
1	E	376	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 PDB entries followed by that with respect to all EM entries.

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	B	267/562 (48%)	266 (100%)	1 (0%)	93 98
1	C	267/562 (48%)	266 (100%)	1 (0%)	93 98
1	D	267/562 (48%)	266 (100%)	1 (0%)	93 98
1	E	267/562 (48%)	266 (100%)	1 (0%)	93 98
All	All	1068/2248 (48%)	1064 (100%)	4 (0%)	94 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	743	ARG
1	B	743	ARG
1	D	743	ARG
1	E	743	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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	$\#\|Z\| > 2$
2	6ET	B	801	-	27,27,27	2.36	6 (22%)	34,37,37	1.97	7 (20%)
2	6ET	C	801	-	27,27,27	2.35	6 (22%)	34,37,37	1.97	7 (20%)
2	6ET	D	801	-	27,27,27	2.35	6 (22%)	34,37,37	1.98	7 (20%)
2	6ET	E	801	-	27,27,27	2.35	6 (22%)	34,37,37	1.97	7 (20%)

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	6ET	B	801	-	-	0/10/20/20	0/2/3/3
2	6ET	C	801	-	-	0/10/20/20	0/2/3/3
2	6ET	D	801	-	-	0/10/20/20	0/2/3/3
2	6ET	E	801	-	-	0/10/20/20	0/2/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	6ET	C14-S15	-5.34	1.59	1.67
2	D	801	6ET	C14-S15	-5.33	1.59	1.67
2	C	801	6ET	C14-S15	-5.33	1.59	1.67
2	E	801	6ET	C14-S15	-5.32	1.59	1.67
2	B	801	6ET	C04-C10	-3.97	1.33	1.40
2	E	801	6ET	C04-C10	-3.96	1.33	1.40
2	D	801	6ET	C04-C10	-3.94	1.33	1.40
2	C	801	6ET	C04-C10	-3.94	1.33	1.40
2	B	801	6ET	C07-N08	-2.70	1.40	1.47
2	C	801	6ET	C07-N08	-2.70	1.40	1.47
2	E	801	6ET	C07-N08	-2.69	1.41	1.47
2	D	801	6ET	C07-N08	-2.66	1.41	1.47
2	D	801	6ET	C09-N08	-2.11	1.42	1.46
2	B	801	6ET	C09-N08	-2.11	1.42	1.46
2	C	801	6ET	C09-N08	-2.10	1.43	1.46
2	E	801	6ET	C09-N08	-2.08	1.43	1.46
2	D	801	6ET	C14-N16	5.59	1.42	1.34
2	B	801	6ET	C14-N16	5.59	1.42	1.34
2	C	801	6ET	C14-N16	5.59	1.42	1.34
2	E	801	6ET	C14-N16	5.63	1.42	1.34
2	D	801	6ET	C14-N08	6.21	1.43	1.33
2	E	801	6ET	C14-N08	6.21	1.43	1.33
2	C	801	6ET	C14-N08	6.21	1.43	1.33
2	B	801	6ET	C14-N08	6.26	1.43	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	801	6ET	C06-C05-C04	-5.67	102.80	113.84
2	E	801	6ET	C06-C05-C04	-5.66	102.83	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	6ET	C06-C05-C04	-5.65	102.84	113.84
2	C	801	6ET	C06-C05-C04	-5.65	102.84	113.84
2	D	801	6ET	C07-N08-C14	-5.15	111.29	121.84
2	E	801	6ET	C07-N08-C14	-5.14	111.30	121.84
2	C	801	6ET	C07-N08-C14	-5.13	111.33	121.84
2	B	801	6ET	C07-N08-C14	-5.12	111.34	121.84
2	C	801	6ET	C09-C10-C04	-3.35	117.61	121.25
2	D	801	6ET	C09-C10-C04	-3.33	117.64	121.25
2	B	801	6ET	C09-C10-C04	-3.29	117.68	121.25
2	E	801	6ET	C09-C10-C04	-3.28	117.68	121.25
2	D	801	6ET	C17-C18-C19	-2.37	107.56	112.83
2	B	801	6ET	C17-C18-C19	-2.36	107.59	112.83
2	E	801	6ET	C17-C18-C19	-2.35	107.61	112.83
2	C	801	6ET	C17-C18-C19	-2.35	107.61	112.83
2	C	801	6ET	C18-C19-C20	-2.13	115.86	121.24
2	E	801	6ET	C18-C19-C20	-2.11	115.90	121.24
2	D	801	6ET	C18-C19-C20	-2.11	115.91	121.24
2	B	801	6ET	C18-C19-C20	-2.10	115.94	121.24
2	C	801	6ET	C03-C04-C10	2.99	122.39	118.81
2	D	801	6ET	C03-C04-C10	2.99	122.40	118.81
2	B	801	6ET	C03-C04-C10	3.00	122.42	118.81
2	E	801	6ET	C03-C04-C10	3.05	122.47	118.81
2	B	801	6ET	C09-C10-C11	3.29	123.37	119.29
2	E	801	6ET	C09-C10-C11	3.32	123.41	119.29
2	C	801	6ET	C09-C10-C11	3.33	123.42	119.29
2	D	801	6ET	C09-C10-C11	3.33	123.42	119.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	6ET	5	0
2	C	801	6ET	5	0
2	D	801	6ET	4	0
2	E	801	6ET	4	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.