wwPDB EM Map/Model Validation Report (i)

Jun 13, 2016 – 04:32 PM EDT

PDB ID	:	5IRX
EMDB ID:	:	EMD-8117
Title	:	Structure of TRPV1 in complex with DkTx and RTX, determined in lipid nanodisc
Authors	:	Gao, Y.; Cao, E.; Julius, D.; Cheng, Y.
Deposited on	:	2016-03-14
Resolution	:	2.95 Å(reported)
Based on PDB ID	:	3J5Q

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

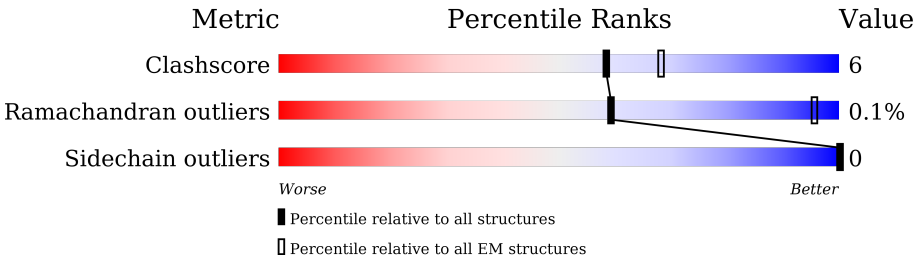
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 2.95 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	A	636	57% 5% 38%
1	B	636	56% 5% 38%
1	C	636	57% 5% 38%
1	D	636	56% 6% 38%
2	E	75	84% 16%
2	F	75	87% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13677 atoms, of which 515 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	A	394	Total	C	N	O	S	0	0
			2893	1920	479	478	16		
1	B	394	Total	C	N	O	S	0	0
			2893	1920	479	478	16		
1	C	394	Total	C	N	O	S	0	0
			2893	1920	479	478	16		
1	D	394	Total	C	N	O	S	0	0
			2893	1920	479	478	16		

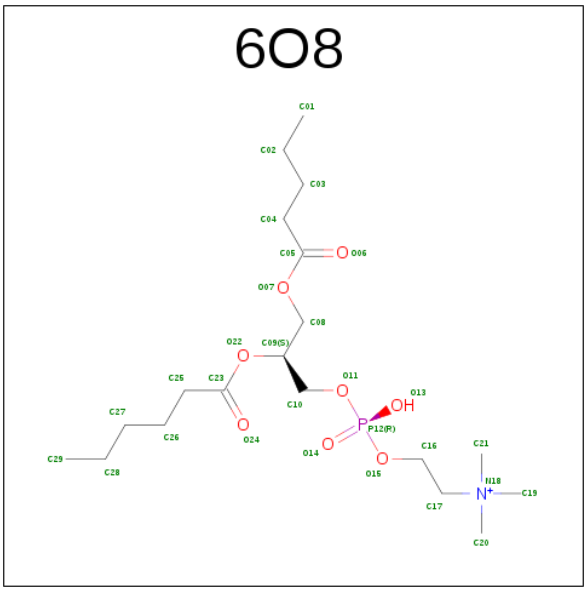
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	ALA	-	expression tag	UNP O35433
A	107	MET	-	expression tag	UNP O35433
A	108	GLY	-	expression tag	UNP O35433
A	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
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
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

- Molecule 2 is a protein called Tau-theraphotoxin-Hs1a.

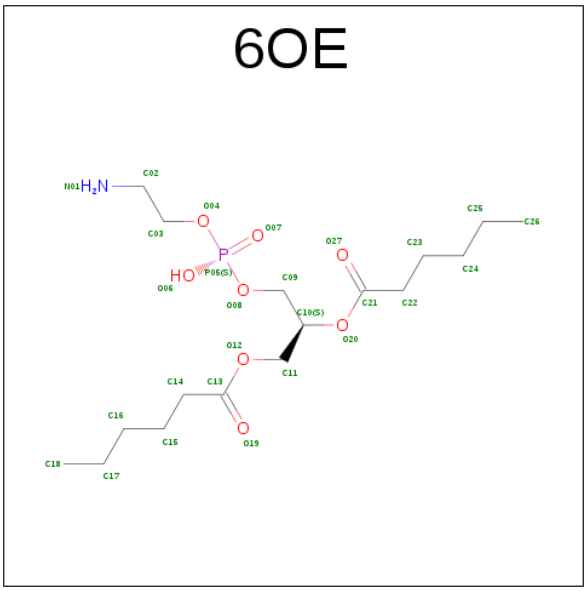
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	75	Total	C	N	O	S	0	0
			493	311	83	86	13		
2	F	75	Total	C	N	O	S	0	0
			493	311	83	86	13		

- Molecule 3 is (4R,7S)-4-hydroxy-N,N,N-trimethyl-4,9-dioxo-7-[(pentanoyloxy)methyl]-3,5,8-trioxa-4lambda 5 -phosphatetradecan-1-aminium (three-letter code: 6O8) (formula: $C_{19}H_{39}NO_8P$).



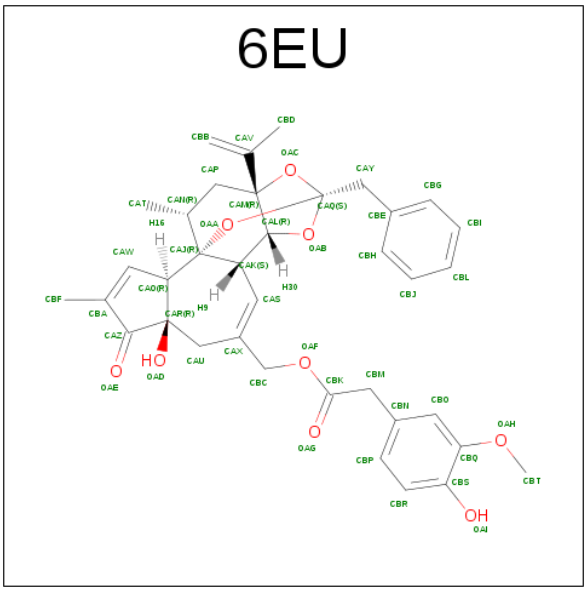
Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			65	19	36	1	8	1	
3	B	1	Total	C	H	N	O	P	0
			65	19	36	1	8	1	
3	C	1	Total	C	H	N	O	P	0
			65	19	36	1	8	1	
3	D	1	Total	C	H	N	O	P	0
			65	19	36	1	8	1	

- Molecule 4 is (2S)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(hexanoyloxy)propyl hexanoate (three-letter code: 6OE) (formula: $C_{17}H_{34}NO_8P$).



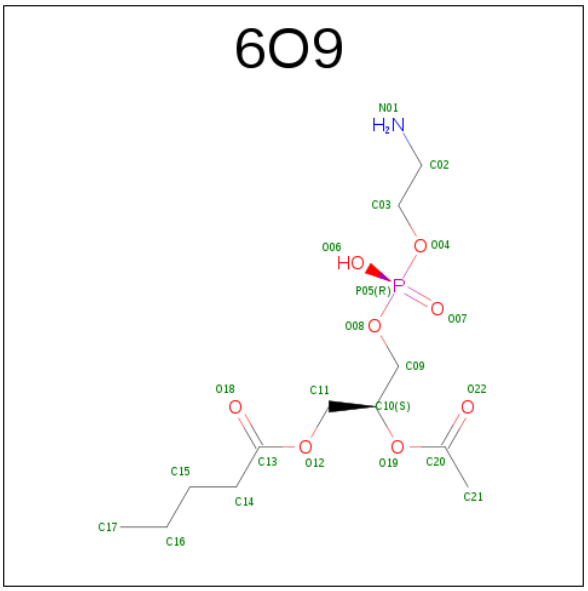
Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	C	H	N	O	P	0
			116	34	62	2	16	2	
4	A	1	Total	C	H	N	O	P	0
			116	34	62	2	16	2	
4	B	1	Total	C	H	N	O	P	0
			58	17	31	1	8	1	
4	C	1	Total	C	H	N	O	P	0
			57	17	30	1	8	1	
4	D	1	Total	C	H	N	O	P	0
			116	34	62	2	16	2	
4	D	1	Total	C	H	N	O	P	0
			116	34	62	2	16	2	
4	E	1	Total	C	H	N	O	P	0
			58	17	31	1	8	1	
4	F	1	Total	C	H	N	O	P	0
			58	17	31	1	8	1	

- Molecule 5 is resiniferatoxin (three-letter code: 6EU) (formula: $C_{37}H_{40}O_9$).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	H	O	0
			56	37	10	9	
5	B	1	Total	C	H	O	0
			56	37	10	9	
5	C	1	Total	C	H	O	0
			56	37	10	9	
5	D	1	Total	C	H	O	0
			56	37	10	9	

- Molecule 6 is (2S)-2-(acetyloxy)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}propyl pentanoate (three-letter code: 6O9) (formula: $C_{12}H_{24}NO_8P$).



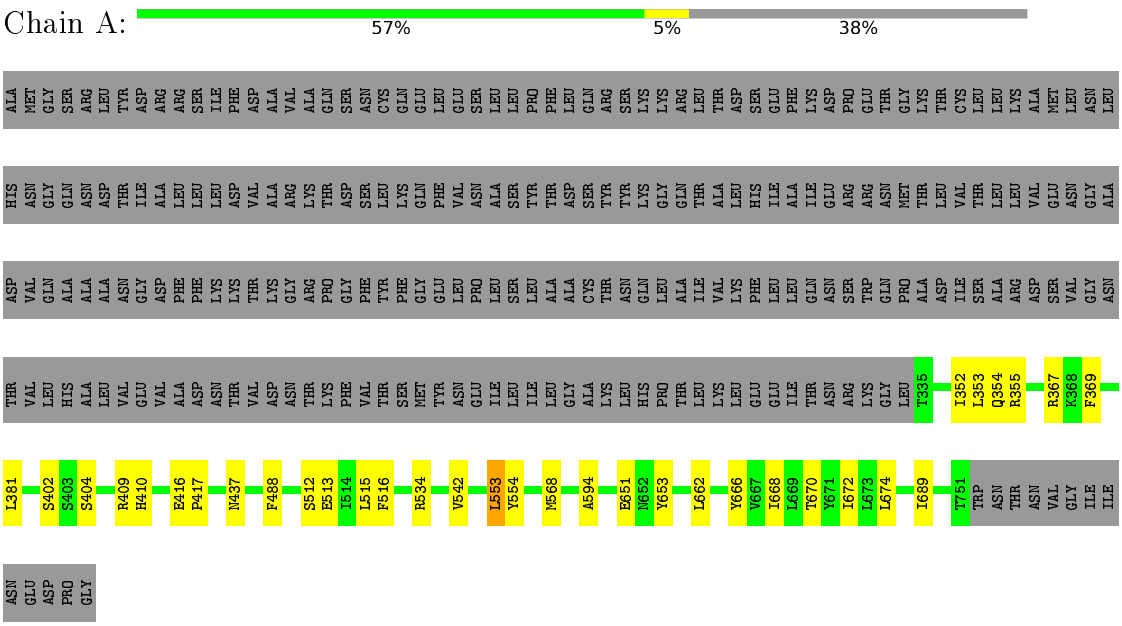
Mol	Chain	Residues	Atoms						AltConf
6	D	1	Total	C	H	N	O	P	0
			43	12	21	1	8	1	
6	E	1	Total	C	H	N	O	P	0
			43	12	21	1	8	1	
6	F	1	Total	C	H	N	O	P	0
			86	24	42	2	16	2	
6	F	1	Total	C	H	N	O	P	0
			86	24	42	2	16	2	

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.

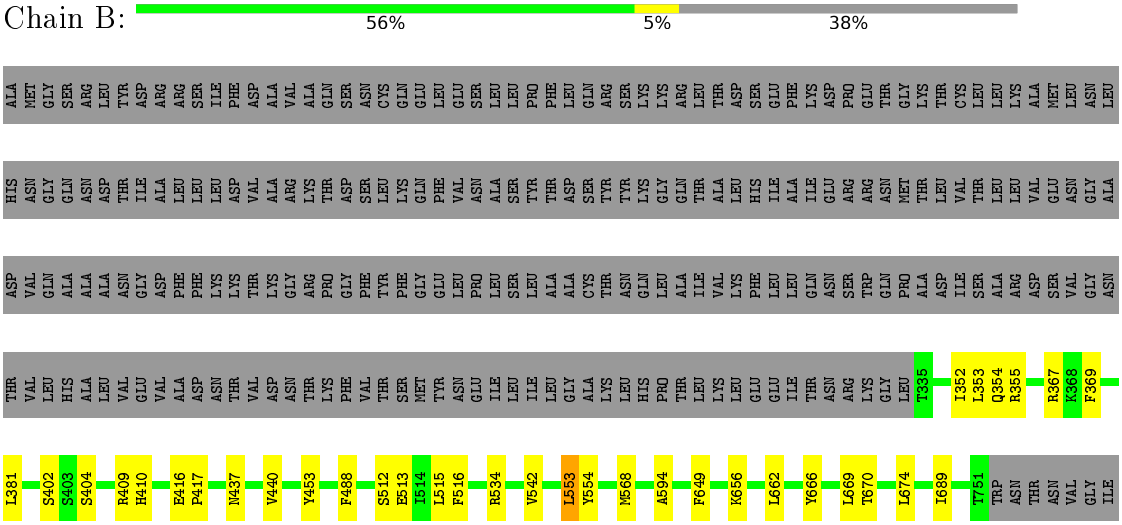
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain A:



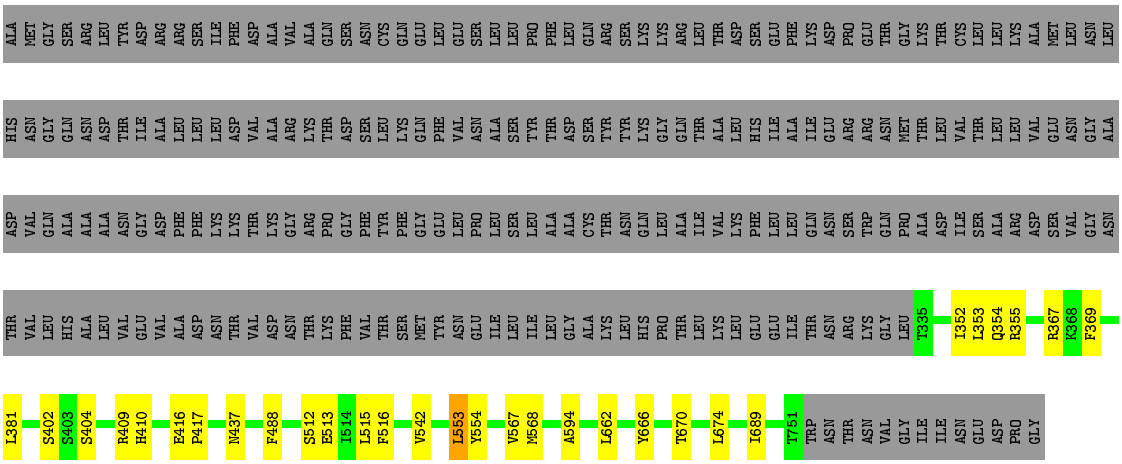
- Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain B:



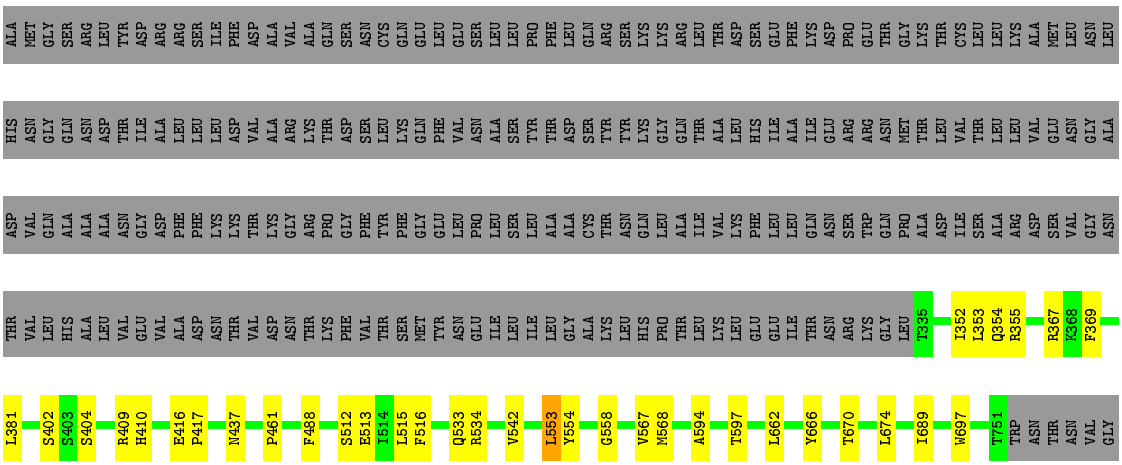
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain C:



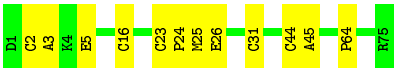
• Molecule 1: Transient receptor potential cation channel subfamily V member 1

Chain D:



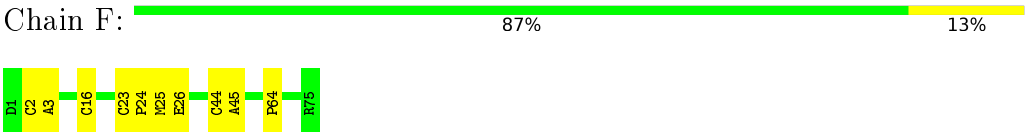
• Molecule 2: Tau-theraphotoxin-Hs1a

Chain E:



• Molecule 2: Tau-theraphotoxin-Hs1a

Chain F:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	73929	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: 6OE, 6EU, 6O8, 6O9

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	A	0.58	0/2966	0.64	1/4034 (0.0%)
1	B	0.58	0/2966	0.64	1/4034 (0.0%)
1	C	0.58	0/2966	0.64	1/4034 (0.0%)
1	D	0.58	0/2966	0.64	1/4034 (0.0%)
2	E	0.49	0/505	0.74	2/688 (0.3%)
2	F	0.49	0/505	0.74	2/688 (0.3%)
All	All	0.57	0/12874	0.65	8/17512 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	23	CYS	C-N-CD	-7.04	105.11	120.60
2	E	23	CYS	C-N-CD	-7.02	105.15	120.60
1	B	553	LEU	CA-CB-CG	5.76	128.55	115.30
1	D	553	LEU	CA-CB-CG	5.76	128.55	115.30
2	F	23	CYS	C-N-CA	5.76	146.19	122.00
2	E	23	CYS	C-N-CA	5.75	146.15	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	553	LEU	CA-CB-CG	5.73	128.49	115.30
1	C	553	LEU	CA-CB-CG	5.73	128.47	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	416	GLU	Peptide
1	B	416	GLU	Peptide
1	C	416	GLU	Peptide
1	D	416	GLU	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	A	2893	0	2601	33	0
1	B	2893	0	2601	35	0
1	C	2893	0	2601	31	0
1	D	2893	0	2601	33	0
2	E	493	0	367	6	0
2	F	493	0	367	5	0
3	A	29	36	0	8	0
3	B	29	36	0	9	0
3	C	29	36	0	8	0
3	D	29	36	0	7	0
4	A	54	62	0	1	0
4	B	27	31	0	1	0
4	C	27	30	0	0	0
4	D	54	62	0	1	0
4	E	27	31	0	1	0
4	F	27	31	0	1	0
5	A	46	10	0	12	0
5	B	46	10	0	10	0
5	C	46	10	0	10	0
5	D	46	10	0	10	0
6	D	22	21	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	22	21	0	0	0
6	F	44	42	0	0	0
All	All	13162	515	11138	146	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 6.

All (146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:26:GLU:O	4:F:103:6OE:O07	1.74	1.05
2:E:26:GLU:O	4:E:102:6OE:O07	1.82	0.96
1:C:513:GLU:OE1	3:C:801:6O8:C21	2.23	0.87
1:D:513:GLU:OE1	3:D:801:6O8:C21	2.25	0.85
1:A:513:GLU:OE1	3:A:801:6O8:C21	2.26	0.84
1:D:513:GLU:OE2	3:D:801:6O8:C21	2.27	0.82
1:C:513:GLU:OE2	3:C:801:6O8:C21	2.29	0.81
1:B:513:GLU:OE1	3:B:801:6O8:C21	2.29	0.81
1:B:554:TYR:HB2	5:B:803:6EU:CBT	2.10	0.80
1:D:488:PHE:CZ	3:D:801:6O8:O24	2.37	0.78
1:A:513:GLU:OE2	3:A:801:6O8:C21	2.32	0.78
1:C:488:PHE:CZ	3:C:801:6O8:O24	2.36	0.78
1:B:513:GLU:OE2	3:B:801:6O8:C21	2.32	0.77
1:A:554:TYR:HB2	5:A:804:6EU:CBT	2.14	0.77
1:A:488:PHE:CZ	3:A:801:6O8:O24	2.38	0.75
1:C:554:TYR:HB2	5:C:803:6EU:CBT	2.17	0.74
1:C:513:GLU:CD	3:C:801:6O8:C21	2.56	0.74
1:D:554:TYR:HB2	5:D:805:6EU:CBT	2.16	0.74
1:D:513:GLU:CD	3:D:801:6O8:C21	2.56	0.74
1:A:513:GLU:CD	3:A:801:6O8:C21	2.59	0.71
1:B:513:GLU:CD	3:B:801:6O8:C21	2.61	0.69
1:B:488:PHE:CZ	3:B:801:6O8:O24	2.45	0.68
1:B:437:ASN:OD1	3:B:801:6O8:O06	2.13	0.66
2:F:44:CYS:SG	2:F:45:ALA:N	2.69	0.65
2:E:2:CYS:SG	2:E:3:ALA:N	2.69	0.65
2:F:2:CYS:SG	2:F:3:ALA:N	2.69	0.65
2:E:44:CYS:SG	2:E:45:ALA:N	2.69	0.65
1:A:437:ASN:OD1	3:A:801:6O8:O06	2.16	0.62
1:C:437:ASN:OD1	3:C:801:6O8:O06	2.16	0.62
1:B:352:ILE:HG23	1:B:355:ARG:HH21	1.66	0.61
1:C:352:ILE:HG23	1:C:355:ARG:HH21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:ILE:HG23	1:D:355:ARG:HH21	1.66	0.60
1:A:516:PHE:CD2	3:A:801:6O8:C19	2.84	0.59
1:C:516:PHE:CD2	3:C:801:6O8:C19	2.86	0.59
1:A:352:ILE:HG23	1:A:355:ARG:HH21	1.66	0.59
1:B:512:SER:OG	5:B:803:6EU:CBT	2.51	0.59
1:D:437:ASN:OD1	3:D:801:6O8:O06	2.21	0.59
1:D:516:PHE:CD2	3:D:801:6O8:C19	2.86	0.58
1:C:353:LEU:HB3	1:C:417:PRO:HG3	1.88	0.56
1:B:353:LEU:HB3	1:B:417:PRO:HG3	1.88	0.55
1:D:353:LEU:HB3	1:D:417:PRO:HG3	1.88	0.55
1:C:512:SER:OG	5:C:803:6EU:CBT	2.54	0.55
1:D:512:SER:OG	5:D:805:6EU:CBT	2.55	0.55
1:A:353:LEU:HB3	1:A:417:PRO:HG3	1.88	0.54
5:C:803:6EU:CAW	5:C:803:6EU:CAT	2.85	0.54
5:A:804:6EU:CAT	5:A:804:6EU:CAW	2.86	0.54
1:B:516:PHE:CD2	3:B:801:6O8:C19	2.91	0.53
5:B:803:6EU:CAT	5:B:803:6EU:CAW	2.86	0.53
5:D:805:6EU:CAT	5:D:805:6EU:CAW	2.86	0.53
1:D:404:SER:H	1:D:409:ARG:HH22	1.57	0.53
1:B:404:SER:H	1:B:409:ARG:HH22	1.57	0.53
1:C:404:SER:H	1:C:409:ARG:HH22	1.57	0.52
1:B:534:ARG:NE	4:B:802:6OE:C11	2.73	0.52
1:A:404:SER:H	1:A:409:ARG:HH22	1.57	0.52
1:A:542:VAL:HG13	1:B:594:ALA:HB1	1.92	0.51
1:C:594:ALA:HB1	1:D:542:VAL:HG13	1.94	0.50
1:A:553:LEU:HD11	5:A:804:6EU:CBN	2.42	0.50
1:A:553:LEU:CD1	5:A:804:6EU:CBP	2.89	0.50
1:B:515:LEU:HD23	5:B:803:6EU:CBB	2.42	0.50
1:B:453:TYR:HA	1:D:597:THR:HG22	1.94	0.50
1:D:568:MET:HB3	1:D:689:ILE:HG21	1.94	0.49
1:A:512:SER:OG	5:A:804:6EU:CBT	2.60	0.49
1:B:402:SER:O	1:B:409:ARG:NH2	2.46	0.49
1:C:402:SER:O	1:C:409:ARG:NH2	2.46	0.49
1:D:402:SER:O	1:D:409:ARG:NH2	2.46	0.49
1:C:568:MET:HB3	1:C:689:ILE:HG21	1.94	0.49
1:B:542:VAL:HG13	1:D:594:ALA:HB1	1.95	0.48
1:A:594:ALA:HB1	1:C:542:VAL:HG13	1.94	0.48
1:A:402:SER:O	1:A:409:ARG:NH2	2.46	0.48
1:B:670:THR:HA	1:B:674:LEU:HB2	1.96	0.48
1:B:568:MET:HB3	1:B:689:ILE:HG21	1.94	0.48
1:A:670:THR:HA	1:A:674:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:CD2	5:A:804:6EU:CBB	2.91	0.48
1:A:553:LEU:HD11	5:A:804:6EU:CBM	2.43	0.48
1:D:670:THR:HA	1:D:674:LEU:HB2	1.96	0.48
1:A:534:ARG:NE	4:A:803:6OE:C11	2.77	0.48
1:C:670:THR:HA	1:C:674:LEU:HB2	1.95	0.47
1:A:568:MET:HB3	1:A:689:ILE:HG21	1.94	0.47
1:A:515:LEU:HD23	5:A:804:6EU:CBB	2.44	0.47
1:B:649:PHE:O	1:B:656:LYS:NZ	2.37	0.47
1:D:534:ARG:NE	4:D:804:6OE:C11	2.78	0.47
1:A:651:GLU:OE2	1:A:653:TYR:OH	2.26	0.46
1:A:554:TYR:CZ	3:A:801:6O8:C20	2.98	0.46
1:B:440:VAL:HG12	3:B:801:6O8:C25	2.45	0.46
1:B:515:LEU:CD2	5:B:803:6EU:CBB	2.93	0.46
1:B:553:LEU:HD11	5:B:803:6EU:CBM	2.45	0.46
1:A:553:LEU:HD11	5:A:804:6EU:CBP	2.45	0.46
1:C:554:TYR:CZ	3:C:801:6O8:C20	2.99	0.46
5:A:804:6EU:CBJ	1:B:669:LEU:HD13	2.46	0.45
1:B:554:TYR:CZ	3:B:801:6O8:C20	2.99	0.45
1:C:553:LEU:HD11	5:C:803:6EU:CBM	2.46	0.45
1:C:553:LEU:HD11	5:C:803:6EU:CBN	2.46	0.45
1:D:553:LEU:HD11	5:D:805:6EU:CBM	2.47	0.45
1:C:515:LEU:CD2	5:C:803:6EU:CBB	2.95	0.44
1:D:553:LEU:HD11	5:D:805:6EU:CBN	2.47	0.44
1:D:553:LEU:CD1	5:D:805:6EU:CBP	2.95	0.44
1:D:515:LEU:CD2	5:D:805:6EU:CBB	2.96	0.44
1:C:409:ARG:HG3	1:C:410:HIS:H	1.83	0.44
1:D:409:ARG:HG3	1:D:410:HIS:H	1.83	0.44
1:C:354:GLN:HE22	1:C:417:PRO:HD3	1.83	0.43
1:D:515:LEU:HD23	5:D:805:6EU:CBB	2.48	0.43
1:B:409:ARG:HG3	1:B:410:HIS:H	1.83	0.43
1:C:515:LEU:HD23	5:C:803:6EU:CBB	2.48	0.43
1:C:553:LEU:CD1	5:C:803:6EU:CBP	2.95	0.43
1:B:553:LEU:CD1	5:B:803:6EU:CBP	2.96	0.43
1:B:512:SER:HB2	5:B:803:6EU:OAI	2.18	0.43
1:B:354:GLN:HE22	1:B:417:PRO:HD3	1.83	0.43
1:B:553:LEU:HD11	5:B:803:6EU:CBN	2.49	0.43
1:A:354:GLN:HE22	1:A:417:PRO:HD3	1.84	0.43
1:A:409:ARG:HG3	1:A:410:HIS:H	1.83	0.43
1:A:662:LEU:O	1:A:666:TYR:N	2.53	0.42
1:D:369:PHE:O	1:D:381:LEU:N	2.51	0.42
1:D:554:TYR:CZ	3:D:801:6O8:C20	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:TYR:CE2	3:A:801:6O8:C20	3.03	0.42
1:B:369:PHE:O	1:B:381:LEU:N	2.51	0.42
1:D:353:LEU:HA	1:D:367:ARG:HG2	2.02	0.42
1:D:354:GLN:HE22	1:D:417:PRO:HD3	1.83	0.42
1:D:662:LEU:O	1:D:666:TYR:N	2.53	0.42
1:C:662:LEU:O	1:C:666:TYR:N	2.53	0.42
1:B:662:LEU:O	1:B:666:TYR:N	2.53	0.42
2:F:2:CYS:SG	2:F:16:CYS:N	2.93	0.42
1:A:353:LEU:HA	1:A:367:ARG:HG2	2.02	0.41
1:A:369:PHE:O	1:A:381:LEU:N	2.51	0.41
1:C:353:LEU:HA	1:C:367:ARG:HG2	2.02	0.41
1:B:353:LEU:HA	1:B:367:ARG:HG2	2.02	0.41
5:A:804:6EU:CBL	1:B:669:LEU:HD13	2.50	0.41
2:E:2:CYS:SG	2:E:16:CYS:N	2.93	0.41
5:B:803:6EU:OAD	5:B:803:6EU:CAK	2.69	0.41
1:C:666:TYR:O	1:C:670:THR:HG22	2.21	0.41
1:B:554:TYR:CE2	3:B:801:6O8:C20	3.04	0.41
2:F:24:PRO:HB2	2:F:25:MET:H	1.76	0.41
1:D:553:LEU:HD11	5:D:805:6EU:CBP	2.51	0.41
1:D:558:GLY:O	1:D:697:TRP:NE1	2.46	0.41
1:D:461:PRO:HA	1:D:533:GLN:HG2	2.03	0.41
1:A:666:TYR:O	1:A:670:THR:HG22	2.21	0.40
1:C:369:PHE:O	1:C:381:LEU:N	2.51	0.40
1:C:553:LEU:HD11	5:C:803:6EU:CBP	2.51	0.40
5:C:803:6EU:CAK	5:C:803:6EU:OAD	2.69	0.40
5:D:805:6EU:OAD	5:D:805:6EU:CAK	2.69	0.40
2:E:24:PRO:HB2	2:E:25:MET:H	1.76	0.40
1:C:554:TYR:CE2	3:C:801:6O8:C20	3.04	0.40
1:A:668:ILE:HD12	1:A:672:ILE:HG13	2.03	0.40
1:D:567:VAL:HG12	1:D:689:ILE:HD11	2.03	0.40
5:A:804:6EU:OAD	5:A:804:6EU:CAK	2.69	0.40
1:C:567:VAL:HG12	1:C:689:ILE:HD11	2.03	0.40
2:E:5:GLU:HA	2:E:31:CYS:HB2	2.02	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	A	392/636 (62%)	355 (91%)	37 (9%)	0	100	100
1	B	392/636 (62%)	356 (91%)	36 (9%)	0	100	100
1	C	392/636 (62%)	355 (91%)	37 (9%)	0	100	100
1	D	392/636 (62%)	355 (91%)	37 (9%)	0	100	100
2	E	73/75 (97%)	54 (74%)	18 (25%)	1 (1%)	14	49
2	F	73/75 (97%)	54 (74%)	18 (25%)	1 (1%)	14	49
All	All	1714/2694 (64%)	1529 (89%)	183 (11%)	2 (0%)	59	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	64	PRO
2	F	64	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	A	242/562 (43%)	242 (100%)	0	100	100
1	B	242/562 (43%)	242 (100%)	0	100	100
1	C	242/562 (43%)	242 (100%)	0	100	100
1	D	242/562 (43%)	242 (100%)	0	100	100
2	E	37/66 (56%)	37 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	37/66 (56%)	37 (100%)	0	100	100
All	All	1042/2380 (44%)	1042 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

20 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	6O8	A	801	-	28,28,28	1.53	7 (25%)	32,36,36	1.32	4 (12%)
4	6OE	A	802	-	25,26,26	1.16	4 (16%)	26,31,31	1.23	2 (7%)
4	6OE	A	803	-	25,26,26	1.16	4 (16%)	26,31,31	1.09	2 (7%)
5	6EU	A	804	-	43,52,52	2.51	11 (25%)	40,83,83	1.49	5 (12%)
3	6O8	B	801	-	28,28,28	1.53	7 (25%)	32,36,36	1.31	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	6OE	B	802	-	25,26,26	1.16	4 (16%)	26,31,31	1.10	2 (7%)
5	6EU	B	803	-	43,52,52	2.52	11 (25%)	40,83,83	1.49	5 (12%)
3	6O8	C	801	-	28,28,28	1.53	7 (25%)	32,36,36	1.32	5 (15%)
4	6OE	C	802	-	25,26,26	1.16	4 (16%)	26,31,31	1.10	2 (7%)
5	6EU	C	803	-	43,52,52	2.51	11 (25%)	40,83,83	1.49	5 (12%)
3	6O8	D	801	-	28,28,28	1.53	7 (25%)	32,36,36	1.31	5 (15%)
6	6O9	D	802	-	20,21,21	1.30	4 (20%)	21,26,26	1.36	2 (9%)
4	6OE	D	803	-	25,26,26	1.16	4 (16%)	26,31,31	1.20	2 (7%)
4	6OE	D	804	-	25,26,26	1.16	4 (16%)	26,31,31	1.09	2 (7%)
5	6EU	D	805	-	43,52,52	2.51	11 (25%)	40,83,83	1.50	5 (12%)
6	6O9	E	101	-	20,21,21	1.32	4 (20%)	21,26,26	1.36	2 (9%)
4	6OE	E	102	-	25,26,26	1.16	4 (16%)	26,31,31	1.21	2 (7%)
6	6O9	F	101	-	20,21,21	1.31	4 (20%)	21,26,26	1.36	2 (9%)
6	6O9	F	102	-	20,21,21	1.31	4 (20%)	21,26,26	1.37	2 (9%)
4	6OE	F	103	-	25,26,26	1.17	4 (16%)	26,31,31	1.21	2 (7%)

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	6O8	A	801	-	-	0/32/32/32	0/0/0/0
4	6OE	A	802	-	-	0/30/30/30	0/0/0/0
4	6OE	A	803	-	-	0/30/30/30	0/0/0/0
5	6EU	A	804	-	-	0/19/101/101	0/4/7/7
3	6O8	B	801	-	-	0/32/32/32	0/0/0/0
4	6OE	B	802	-	-	0/30/30/30	0/0/0/0
5	6EU	B	803	-	-	0/19/101/101	0/4/7/7
3	6O8	C	801	-	-	0/32/32/32	0/0/0/0
4	6OE	C	802	-	-	0/30/30/30	0/0/0/0
5	6EU	C	803	-	-	0/19/101/101	0/4/7/7
3	6O8	D	801	-	-	0/32/32/32	0/0/0/0
6	6O9	D	802	-	-	0/24/24/24	0/0/0/0
4	6OE	D	803	-	-	0/30/30/30	0/0/0/0
4	6OE	D	804	-	-	0/30/30/30	0/0/0/0
5	6EU	D	805	-	-	0/19/101/101	0/4/7/7
6	6O9	E	101	-	-	0/24/24/24	0/0/0/0
4	6OE	E	102	-	-	0/30/30/30	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	6O9	F	101	-	-	0/24/24/24	0/0/0/0
6	6O9	F	102	-	-	0/24/24/24	0/0/0/0
4	6OE	F	103	-	-	0/30/30/30	0/0/0/0

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	803	6EU	CAY-CBE	-7.93	1.38	1.51
5	D	805	6EU	CAY-CBE	-7.85	1.39	1.51
5	A	804	6EU	CAY-CBE	-7.85	1.39	1.51
5	C	803	6EU	CAY-CBE	-7.85	1.39	1.51
5	B	803	6EU	CBM-CBN	-7.25	1.39	1.51
5	D	805	6EU	CBM-CBN	-7.25	1.39	1.51
5	A	804	6EU	CBM-CBN	-7.25	1.39	1.51
5	C	803	6EU	CBM-CBN	-7.21	1.39	1.51
5	B	803	6EU	CAR-CAZ	-5.62	1.37	1.53
5	A	804	6EU	CAR-CAZ	-5.62	1.37	1.53
5	C	803	6EU	CAR-CAZ	-5.62	1.37	1.53
5	D	805	6EU	CAR-CAZ	-5.60	1.37	1.53
5	B	803	6EU	CBC-CAX	-4.90	1.38	1.51
5	D	805	6EU	CBC-CAX	-4.88	1.39	1.51
5	A	804	6EU	CBC-CAX	-4.88	1.39	1.51
5	C	803	6EU	CBC-CAX	-4.88	1.39	1.51
5	C	803	6EU	CAZ-CBA	-4.86	1.33	1.46
5	B	803	6EU	CAZ-CBA	-4.85	1.33	1.46
5	D	805	6EU	CAZ-CBA	-4.85	1.33	1.46
5	A	804	6EU	CAZ-CBA	-4.85	1.33	1.46
5	D	805	6EU	CAK-CAS	-4.10	1.40	1.50
5	B	803	6EU	CAK-CAS	-4.09	1.40	1.50
5	A	804	6EU	CAK-CAS	-4.09	1.40	1.50
5	C	803	6EU	CAK-CAS	-4.09	1.40	1.50
3	D	801	6O8	C19-N18	-2.87	1.41	1.50
3	A	801	6O8	C19-N18	-2.85	1.41	1.50
3	C	801	6O8	C19-N18	-2.85	1.41	1.50
3	B	801	6O8	C19-N18	-2.82	1.41	1.50
3	B	801	6O8	O22-C09	-2.77	1.39	1.46
3	D	801	6O8	O22-C09	-2.73	1.39	1.46
3	A	801	6O8	O22-C09	-2.72	1.39	1.46
3	C	801	6O8	O22-C09	-2.72	1.39	1.46
3	A	801	6O8	C17-N18	-2.69	1.42	1.51
3	A	801	6O8	C21-N18	-2.69	1.42	1.50
3	B	801	6O8	C17-N18	-2.68	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	801	6O8	C21-N18	-2.67	1.42	1.50
3	B	801	6O8	C21-N18	-2.67	1.42	1.50
3	D	801	6O8	C17-N18	-2.67	1.42	1.51
3	C	801	6O8	C17-N18	-2.67	1.42	1.51
5	B	803	6EU	CAU-CAX	-2.66	1.40	1.52
5	A	804	6EU	CAU-CAX	-2.66	1.40	1.52
5	C	803	6EU	CAU-CAX	-2.66	1.40	1.52
3	D	801	6O8	C21-N18	-2.65	1.42	1.50
5	D	805	6EU	CAU-CAX	-2.65	1.40	1.52
3	D	801	6O8	O07-C08	-2.65	1.39	1.45
3	A	801	6O8	O07-C08	-2.65	1.39	1.45
3	D	801	6O8	C20-N18	-2.64	1.42	1.50
3	C	801	6O8	C20-N18	-2.64	1.42	1.50
3	B	801	6O8	C20-N18	-2.64	1.42	1.50
3	C	801	6O8	O07-C08	-2.62	1.39	1.45
3	A	801	6O8	C20-N18	-2.62	1.42	1.50
3	B	801	6O8	O07-C08	-2.62	1.39	1.45
6	E	101	6O9	O12-C11	-2.39	1.39	1.45
6	F	101	6O9	O12-C11	-2.37	1.39	1.45
4	C	802	6OE	O20-C10	-2.37	1.40	1.46
4	B	802	6OE	O20-C10	-2.35	1.40	1.46
6	F	102	6O9	O12-C11	-2.35	1.40	1.45
6	D	802	6O9	O12-C11	-2.35	1.40	1.45
4	D	804	6OE	O20-C10	-2.35	1.40	1.46
6	F	101	6O9	O19-C10	-2.35	1.40	1.46
6	F	102	6O9	O19-C10	-2.34	1.40	1.46
6	E	101	6O9	O19-C10	-2.33	1.40	1.46
4	A	803	6OE	O20-C10	-2.33	1.40	1.46
5	B	803	6EU	CAO-CAW	-2.33	1.40	1.49
5	A	804	6EU	CAO-CAW	-2.33	1.40	1.49
5	C	803	6EU	CAO-CAW	-2.32	1.40	1.49
4	E	102	6OE	O12-C11	-2.31	1.40	1.45
4	F	103	6OE	O12-C11	-2.31	1.40	1.45
6	D	802	6O9	O19-C10	-2.31	1.40	1.46
5	D	805	6EU	CAO-CAW	-2.30	1.40	1.49
4	F	103	6OE	O20-C10	-2.27	1.40	1.46
4	A	802	6OE	O12-C11	-2.27	1.40	1.45
4	D	804	6OE	O12-C11	-2.27	1.40	1.45
4	B	802	6OE	O12-C11	-2.27	1.40	1.45
4	D	803	6OE	O12-C11	-2.26	1.40	1.45
4	D	803	6OE	O20-C10	-2.26	1.40	1.46
4	A	803	6OE	O12-C11	-2.25	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	802	6OE	O12-C11	-2.24	1.40	1.45
4	E	102	6OE	O20-C10	-2.23	1.40	1.46
4	A	802	6OE	O20-C10	-2.23	1.40	1.46
4	C	802	6OE	O20-C21	2.01	1.40	1.34
4	D	804	6OE	O20-C21	2.01	1.40	1.34
4	B	802	6OE	O20-C21	2.01	1.40	1.34
4	A	803	6OE	O20-C21	2.03	1.40	1.34
3	A	801	6O8	O07-C05	2.09	1.39	1.33
3	C	801	6O8	O07-C05	2.10	1.39	1.33
4	F	103	6OE	O20-C21	2.10	1.40	1.34
3	B	801	6O8	O07-C05	2.11	1.39	1.33
3	D	801	6O8	O07-C05	2.12	1.39	1.33
4	E	102	6OE	O20-C21	2.12	1.40	1.34
4	D	803	6OE	O20-C21	2.13	1.40	1.34
4	A	802	6OE	O20-C21	2.15	1.40	1.34
6	D	802	6O9	O12-C13	2.27	1.40	1.33
6	F	101	6O9	O12-C13	2.28	1.40	1.33
6	F	102	6O9	O12-C13	2.28	1.40	1.33
6	E	101	6O9	O12-C13	2.29	1.40	1.33
4	E	102	6OE	O12-C13	2.31	1.40	1.33
4	A	802	6OE	O12-C13	2.32	1.40	1.33
4	D	804	6OE	O12-C13	2.33	1.40	1.33
4	A	803	6OE	O12-C13	2.34	1.40	1.33
4	F	103	6OE	O12-C13	2.34	1.40	1.33
4	B	802	6OE	O12-C13	2.35	1.40	1.33
4	D	803	6OE	O12-C13	2.35	1.40	1.33
4	C	802	6OE	O12-C13	2.35	1.40	1.33
6	F	101	6O9	O19-C20	2.38	1.40	1.35
6	D	802	6O9	O19-C20	2.39	1.40	1.35
6	E	101	6O9	O19-C20	2.43	1.40	1.35
6	F	102	6O9	O19-C20	2.43	1.40	1.35
5	B	803	6EU	CAM-CAL	2.61	1.57	1.54
5	D	805	6EU	CAM-CAL	2.62	1.57	1.54
5	A	804	6EU	CAM-CAL	2.64	1.57	1.54
5	C	803	6EU	CAM-CAL	2.64	1.57	1.54
5	A	804	6EU	CBB-CAV	3.08	1.52	1.35
5	B	803	6EU	CBB-CAV	3.08	1.52	1.35
5	C	803	6EU	CBB-CAV	3.08	1.52	1.35
5	D	805	6EU	CBB-CAV	3.09	1.52	1.35
5	B	803	6EU	CAS-CAX	4.46	1.40	1.32
5	D	805	6EU	CAS-CAX	4.46	1.40	1.32
5	A	804	6EU	CAS-CAX	4.46	1.40	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	803	6EU	CAS-CAX	4.46	1.40	1.32

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	805	6EU	CBT-OAH-CBQ	-5.89	108.93	117.53
5	A	804	6EU	CBT-OAH-CBQ	-5.86	108.97	117.53
5	B	803	6EU	CBT-OAH-CBQ	-5.86	108.98	117.53
5	C	803	6EU	CBT-OAH-CBQ	-5.86	108.98	117.53
5	D	805	6EU	CBF-CBA-CAW	-3.40	123.78	130.44
5	A	804	6EU	CBF-CBA-CAW	-3.40	123.78	130.44
5	B	803	6EU	CBF-CBA-CAW	-3.40	123.79	130.44
5	C	803	6EU	CBF-CBA-CAW	-3.38	123.82	130.44
3	C	801	6O8	C09-O22-C23	-2.51	111.71	117.91
3	A	801	6O8	C09-O22-C23	-2.51	111.71	117.91
3	D	801	6O8	C09-O22-C23	-2.49	111.75	117.91
3	B	801	6O8	C09-O22-C23	-2.48	111.78	117.91
5	B	803	6EU	CAO-CAW-CBA	-2.17	107.76	113.34
5	A	804	6EU	CAO-CAW-CBA	-2.17	107.76	113.34
5	D	805	6EU	CAO-CAW-CBA	-2.17	107.76	113.34
5	C	803	6EU	CAO-CAW-CBA	-2.16	107.77	113.34
3	D	801	6O8	P12-O15-C16	-2.06	110.83	121.60
3	C	801	6O8	P12-O15-C16	-2.06	110.83	121.60
3	B	801	6O8	P12-O15-C16	-2.06	110.83	121.60
3	A	801	6O8	P12-O15-C16	-2.06	110.83	121.60
5	C	803	6EU	CBC-OAF-CBK	-2.05	111.21	115.91
5	B	803	6EU	CBC-OAF-CBK	-2.04	111.22	115.91
5	A	804	6EU	CBC-OAF-CBK	-2.03	111.24	115.91
5	D	805	6EU	CBC-OAF-CBK	-2.02	111.28	115.91
3	B	801	6O8	C08-O07-C05	-2.01	111.01	117.00
3	C	801	6O8	C08-O07-C05	-2.01	111.02	117.00
3	D	801	6O8	C08-O07-C05	-2.01	111.02	117.00
6	F	102	6O9	O12-C13-C14	2.37	119.15	111.85
6	D	802	6O9	O12-C13-C14	2.39	119.21	111.85
6	F	101	6O9	O12-C13-C14	2.40	119.22	111.85
6	E	101	6O9	O12-C13-C14	2.42	119.29	111.85
3	D	801	6O8	O07-C05-C04	2.54	119.67	111.85
3	C	801	6O8	O07-C05-C04	2.54	119.67	111.85
3	B	801	6O8	O07-C05-C04	2.55	119.69	111.85
3	A	801	6O8	O07-C05-C04	2.57	119.75	111.85
4	D	804	6OE	O12-C13-C14	2.71	120.20	111.85
4	A	803	6OE	O12-C13-C14	2.72	120.22	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	802	6OE	O12-C13-C14	2.72	120.23	111.85
4	B	802	6OE	O12-C13-C14	2.74	120.27	111.85
4	D	803	6OE	O12-C13-C14	2.74	120.29	111.85
4	E	102	6OE	O12-C13-C14	2.75	120.32	111.85
4	F	103	6OE	O12-C13-C14	2.76	120.34	111.85
4	A	802	6OE	O12-C13-C14	2.77	120.38	111.85
5	C	803	6EU	OAF-CBK-CBM	2.92	115.68	110.63
5	B	803	6EU	OAF-CBK-CBM	2.93	115.70	110.63
5	A	804	6EU	OAF-CBK-CBM	2.94	115.71	110.63
5	D	805	6EU	OAF-CBK-CBM	2.94	115.72	110.63
4	A	803	6OE	O20-C21-C22	3.73	119.38	111.53
4	D	804	6OE	O20-C21-C22	3.75	119.43	111.53
4	B	802	6OE	O20-C21-C22	3.76	119.45	111.53
4	C	802	6OE	O20-C21-C22	3.80	119.52	111.53
4	D	803	6OE	O20-C21-C22	4.35	120.68	111.53
4	E	102	6OE	O20-C21-C22	4.37	120.72	111.53
4	F	103	6OE	O20-C21-C22	4.37	120.74	111.53
4	A	802	6OE	O20-C21-C22	4.44	120.89	111.53
3	D	801	6O8	O22-C23-C25	4.67	121.36	111.53
3	B	801	6O8	O22-C23-C25	4.67	121.36	111.53
3	A	801	6O8	O22-C23-C25	4.69	121.41	111.53
3	C	801	6O8	O22-C23-C25	4.69	121.41	111.53
6	E	101	6O9	O19-C20-C21	4.73	120.08	111.09
6	F	101	6O9	O19-C20-C21	4.75	120.13	111.09
6	D	802	6O9	O19-C20-C21	4.76	120.14	111.09
6	F	102	6O9	O19-C20-C21	4.81	120.24	111.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 79 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	6O8	8	0
4	A	803	6OE	1	0
5	A	804	6EU	12	0
3	B	801	6O8	9	0
4	B	802	6OE	1	0
5	B	803	6EU	10	0
3	C	801	6O8	8	0
5	C	803	6EU	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	801	6O8	7	0
4	D	804	6OE	1	0
5	D	805	6EU	10	0
4	E	102	6OE	1	0
4	F	103	6OE	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.