wwPDB EM Map/Model Validation Report (i)

Aug 29, 2016 – 02:47 PM EDT

PDB ID	:	5SY1
EMDB ID:	:	EMD-8315
Title	:	Structure of the STRA6 receptor for retinol uptake in complex with calmodulin
Authors	:	Clarke, O.B.; Chen, Y.; Mancia, F.
Deposited on	:	2016-08-10
Resolution	:	3.90 Å(reported)

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

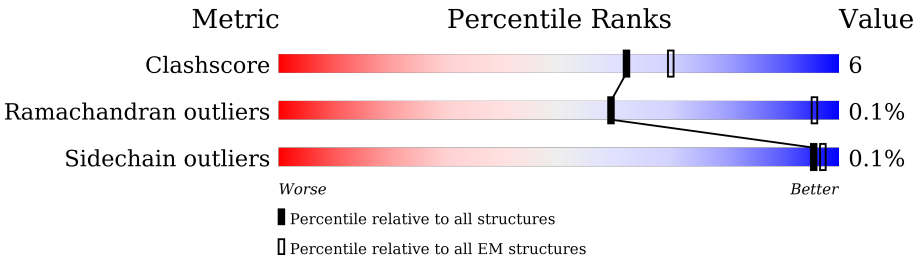
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 3.90 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	C	149	93% 6% .
1	D	149	92% 7% .
2	A	670	76% 11% 13%
2	B	670	75% 11% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11462 atoms, of which 0 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 Calmodulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	147	Total	C	N	O	S	0	0
			1154	707	185	253	9		
1	D	147	Total	C	N	O	S	0	0
			1154	707	185	253	9		

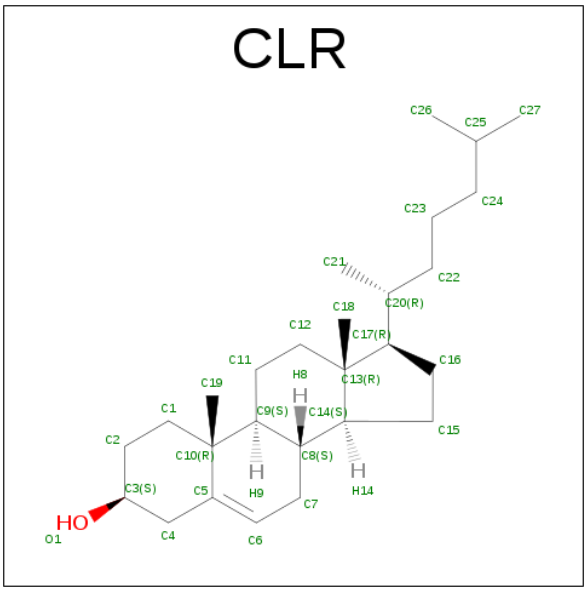
- Molecule 2 is a protein called STRA6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	582	Total	C	N	O	S	0	0
			4545	3002	758	759	26		
2	B	582	Total	C	N	O	S	0	0
			4545	3002	758	759	26		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
3	D	4	Total	Ca	0
			4	4	
3	C	4	Total	Ca	0
			4	4	

- Molecule 4 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



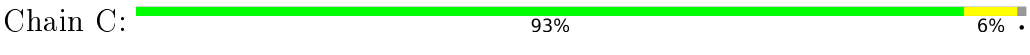
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	

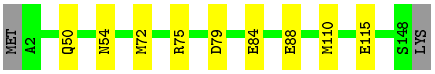
3 Residue-property plots (i)

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: Calmodulin

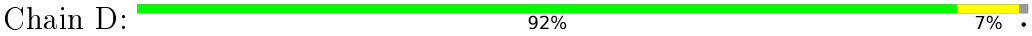
Chain C:





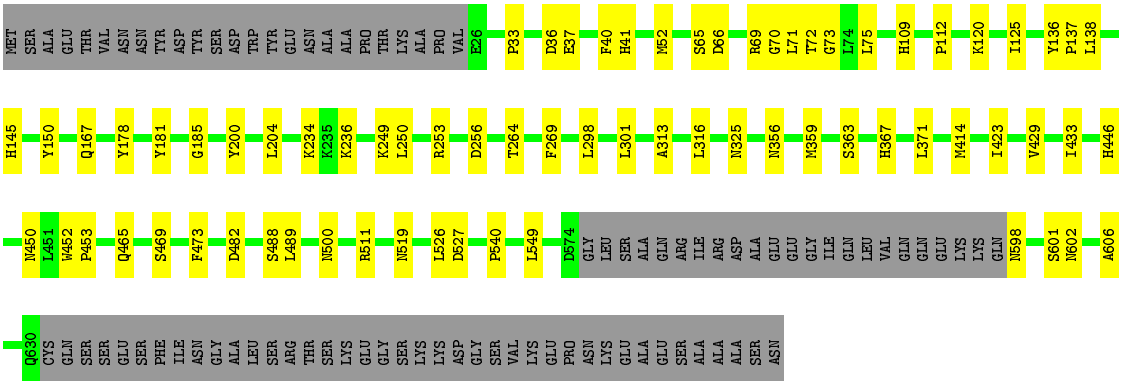
- Molecule 1: Calmodulin

Chain D:



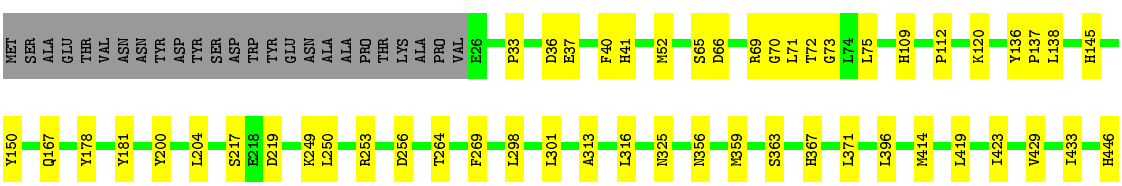
- Molecule 2: STRA6

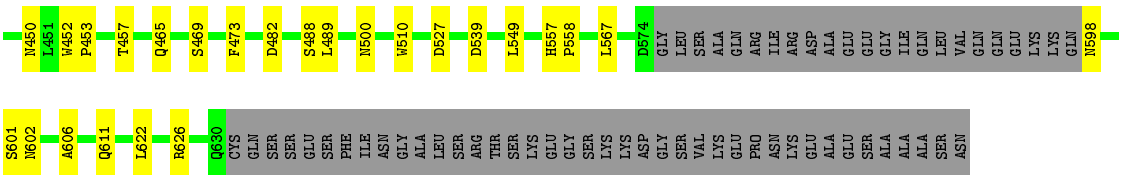
Chain A:



- Molecule 2: STRA6

Chain B:




N450 L451 W452 P453 T457 Q465 S469 F473 D482 S488 L489 N500 W510 D527 D539 L549 H557 P558 L567 D574 GLY LEU SER ALA GLN ARG ILE ARG ASP ALA GLU GLU GLY ILE GLN LEU VAL GLN GLU LYS LYS GLN N598
S601 N602 A606 Q611 L622 R626 Q630 CYS GLN SER SER GLU SER PHE ILE ASN GLY ALA LEU SER ARG THR SER LYS GLU GLY SER LYS LYS ASP GLY SER VAL LYS GLU PRO ASN LYS GLU ALA GLU SER ALA ALA ALA SER ASN

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	56615	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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: CA, CLR

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	C	0.35	0/1166	0.52	0/1566
1	D	0.35	0/1166	0.53	0/1566
2	A	0.42	0/4657	0.58	0/6341
2	B	0.42	0/4657	0.58	0/6341
All	All	0.41	0/11646	0.57	0/15814

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
2	A	0	4
2	B	0	4
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	109	HIS	Peptide
2	A	112	PRO	Peptide
2	A	264	THR	Peptide
2	A	325	ASN	Peptide
2	B	109	HIS	Peptide
2	B	112	PRO	Peptide
2	B	264	THR	Peptide

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Mol	Chain	Res	Type	Group
2	B	325	ASN	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	C	1154	0	1079	6	0
1	D	1154	0	1079	9	0
2	A	4545	0	4663	47	0
2	B	4545	0	4663	51	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	28	0	46	14	0
4	B	28	0	46	15	0
All	All	11462	0	11576	127	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 (127) 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)
4:A:701:CLR:H183	4:A:701:CLR:H222	1.38	1.06
4:B:701:CLR:H222	4:B:701:CLR:H183	1.38	1.04
4:A:701:CLR:H231	4:A:701:CLR:H121	1.48	0.94
4:B:701:CLR:H121	4:B:701:CLR:H231	1.47	0.93
4:A:701:CLR:H121	4:A:701:CLR:C23	2.07	0.83
4:B:701:CLR:H121	4:B:701:CLR:C23	2.08	0.83
4:B:701:CLR:H213	4:B:701:CLR:H181	1.63	0.81
4:B:701:CLR:C12	4:B:701:CLR:H231	2.10	0.81
4:A:701:CLR:H121	4:A:701:CLR:H25	1.61	0.81
4:B:701:CLR:H25	4:B:701:CLR:H121	1.62	0.80
4:A:701:CLR:H213	4:A:701:CLR:H181	1.63	0.80
4:A:701:CLR:H231	4:A:701:CLR:C12	2.11	0.79
4:B:701:CLR:H213	4:B:701:CLR:C18	2.18	0.74
4:A:701:CLR:C18	4:A:701:CLR:H213	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:701:CLR:C25	4:A:701:CLR:H121	2.24	0.67
4:B:701:CLR:C25	4:B:701:CLR:H121	2.26	0.66
2:A:178:TYR:HB3	2:A:181:TYR:HB2	1.79	0.64
2:B:356:ASN:ND2	2:B:414:MET:SD	2.71	0.63
2:B:178:TYR:HB3	2:B:181:TYR:HB2	1.79	0.63
2:B:69:ARG:HG3	2:B:71:LEU:H	1.64	0.63
2:A:69:ARG:NH1	2:B:488:SER:OG	2.32	0.63
2:A:69:ARG:HG3	2:A:71:LEU:H	1.64	0.62
2:A:356:ASN:ND2	2:A:414:MET:SD	2.71	0.61
2:A:249:LYS:HG2	2:A:250:LEU:HG	1.82	0.61
2:B:249:LYS:HG2	2:B:250:LEU:HG	1.82	0.61
2:A:125:ILE:HG21	2:B:457:THR:HG21	1.84	0.60
2:B:217:SER:OG	1:D:42:GLN:NE2	2.36	0.59
1:D:72:MET:SD	1:D:75:ARG:NH1	2.76	0.59
2:B:219:ASP:OD1	1:D:42:GLN:NE2	2.36	0.58
2:A:70:GLY:H	2:B:488:SER:HB2	1.66	0.58
1:C:72:MET:SD	1:C:75:ARG:NH1	2.76	0.58
2:A:69:ARG:HB3	2:A:73:GLY:H	1.69	0.58
2:B:69:ARG:HB3	2:B:73:GLY:H	1.69	0.58
4:A:701:CLR:H272	4:B:701:CLR:H14	1.86	0.57
4:A:701:CLR:H14	4:B:701:CLR:H272	1.86	0.57
1:C:110:MET:HB3	1:C:115:GLU:HA	1.87	0.57
2:A:423:ILE:O	2:A:423:ILE:HG22	2.05	0.56
1:D:110:MET:HB3	1:D:115:GLU:HA	1.87	0.56
2:A:488:SER:OG	2:B:69:ARG:NH1	2.39	0.56
1:D:84:GLU:O	1:D:88:GLU:N	2.40	0.55
2:A:488:SER:HB2	2:B:70:GLY:H	1.71	0.55
4:B:701:CLR:H222	4:B:701:CLR:C18	2.19	0.54
2:B:363:SER:O	2:B:367:HIS:ND1	2.38	0.54
2:A:446:HIS:O	2:A:450:ASN:ND2	2.40	0.54
2:B:446:HIS:O	2:B:450:ASN:ND2	2.40	0.54
1:C:84:GLU:O	1:C:88:GLU:N	2.40	0.54
2:A:138:LEU:O	2:A:200:TYR:OH	2.25	0.52
2:A:363:SER:O	2:A:367:HIS:ND1	2.38	0.52
2:B:423:ILE:O	2:B:423:ILE:HG22	2.09	0.52
1:D:50:GLN:O	1:D:54:ASN:ND2	2.43	0.52
4:A:701:CLR:C18	4:A:701:CLR:C21	2.86	0.51
1:C:50:GLN:O	1:C:54:ASN:ND2	2.43	0.51
2:B:469:SER:HA	2:B:473:PHE:HD2	1.76	0.51
2:B:602:ASN:O	2:B:606:ALA:N	2.44	0.50
1:D:110:MET:O	1:D:115:GLU:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:33:PRO:O	2:A:37:GLU:N	2.45	0.50
2:B:37:GLU:OE1	2:B:167:GLN:NE2	2.45	0.50
2:A:65:SER:OG	2:A:66:ASP:N	2.44	0.50
2:A:465:GLN:HE22	2:A:500:ASN:HD21	1.61	0.49
2:B:482:ASP:N	2:B:482:ASP:OD1	2.37	0.49
1:C:110:MET:O	1:C:115:GLU:N	2.45	0.49
2:B:33:PRO:O	2:B:37:GLU:N	2.45	0.49
2:B:138:LEU:O	2:B:200:TYR:OH	2.25	0.49
2:A:37:GLU:OE1	2:A:167:GLN:NE2	2.45	0.49
2:A:598:ASN:N	2:A:601:SER:HG	2.11	0.48
2:B:65:SER:OG	2:B:66:ASP:N	2.44	0.48
2:A:37:GLU:O	2:A:41:HIS:ND1	2.46	0.48
2:B:359:MET:O	2:B:363:SER:N	2.43	0.48
2:B:465:GLN:HE22	2:B:500:ASN:HD21	1.61	0.48
2:B:598:ASN:N	2:B:601:SER:HG	2.11	0.48
2:B:419:LEU:HD12	2:B:419:LEU:O	2.14	0.48
2:B:150:TYR:HB2	2:B:204:LEU:HD13	1.96	0.47
2:A:298:LEU:HD23	2:A:301:LEU:HD12	1.97	0.47
4:A:701:CLR:H212	4:A:701:CLR:H162	1.68	0.47
2:A:269:PHE:HZ	2:A:371:LEU:HD23	1.80	0.47
2:A:469:SER:HA	2:A:473:PHE:HD2	1.76	0.47
2:A:482:ASP:OD1	2:A:482:ASP:N	2.37	0.47
2:B:298:LEU:HD23	2:B:301:LEU:HD12	1.97	0.47
2:B:37:GLU:O	2:B:41:HIS:ND1	2.46	0.47
2:B:527:ASP:N	2:B:527:ASP:OD1	2.42	0.47
4:A:701:CLR:C22	4:A:701:CLR:H121	2.45	0.47
2:A:253:ARG:NH2	2:A:256:ASP:OD2	2.47	0.47
2:A:602:ASN:O	2:A:606:ALA:N	2.45	0.47
4:B:701:CLR:H121	4:B:701:CLR:C22	2.45	0.47
2:A:150:TYR:HB2	2:A:204:LEU:HD13	1.96	0.46
2:B:567:LEU:HB3	1:D:52:MET:HE3	1.98	0.46
2:A:359:MET:O	2:A:363:SER:N	2.43	0.46
2:B:253:ARG:NH2	2:B:256:ASP:OD2	2.47	0.46
4:B:701:CLR:H212	4:B:701:CLR:H162	1.68	0.46
2:B:269:PHE:HZ	2:B:371:LEU:HD23	1.80	0.46
4:B:701:CLR:C22	4:B:701:CLR:C18	2.86	0.46
1:C:79:ASP:OD2	2:A:234:LYS:NZ	2.49	0.46
2:B:611:GLN:OE1	1:D:75:ARG:NE	2.48	0.46
2:A:527:ASP:N	2:A:527:ASP:OD1	2.42	0.45
2:A:511:ARG:NH1	2:B:539:ASP:OD2	2.51	0.44
2:A:371:LEU:HD13	2:A:549:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLU:HA	2:B:40:PHE:HB2	1.99	0.43
2:B:52:MET:HG3	2:B:137:PRO:HG3	2.01	0.43
2:B:313:ALA:HA	2:B:316:LEU:HB2	2.00	0.43
2:A:52:MET:HG3	2:A:137:PRO:HG3	2.01	0.43
4:A:701:CLR:C12	4:A:701:CLR:H25	2.41	0.43
2:B:452:TRP:CD1	2:B:453:PRO:HD3	2.54	0.43
2:A:145:HIS:ND1	2:A:150:TYR:OH	2.52	0.42
2:A:75:LEU:O	2:A:136:TYR:OH	2.37	0.42
2:B:145:HIS:ND1	2:B:150:TYR:OH	2.52	0.42
2:A:313:ALA:HA	2:A:316:LEU:HB2	2.00	0.42
2:A:452:TRP:CD1	2:A:453:PRO:HD3	2.54	0.42
2:B:37:GLU:HG3	2:B:41:HIS:CE1	2.54	0.42
4:B:701:CLR:H25	4:B:701:CLR:C12	2.42	0.42
2:A:236:LYS:HB3	2:A:236:LYS:HE2	1.81	0.42
2:A:37:GLU:HA	2:A:40:PHE:HB2	2.00	0.42
2:A:489:LEU:HD11	2:B:396:LEU:HD21	2.00	0.42
2:B:36:ASP:O	2:B:40:PHE:N	2.43	0.42
2:B:557:HIS:HA	2:B:558:PRO:HD3	1.89	0.42
2:A:37:GLU:HG3	2:A:41:HIS:CE1	2.54	0.42
2:B:371:LEU:HD13	2:B:549:LEU:HD11	2.00	0.41
2:B:75:LEU:O	2:B:136:TYR:OH	2.37	0.41
2:A:36:ASP:O	2:A:40:PHE:N	2.43	0.41
2:B:473:PHE:CG	2:B:489:LEU:HD12	2.56	0.41
2:B:69:ARG:HG3	2:B:72:THR:H	1.85	0.41
2:A:429:VAL:HA	2:A:433:ILE:HB	2.03	0.41
2:A:540:PRO:HG3	2:B:510:TRP:HD1	1.85	0.41
2:A:69:ARG:HG3	2:A:72:THR:H	1.85	0.41
2:B:622:LEU:O	2:B:626:ARG:N	2.54	0.41
2:A:181:TYR:O	2:A:185:GLY:N	2.51	0.40
2:B:429:VAL:HA	2:B:433:ILE:HB	2.03	0.40
2:A:526:LEU:HD23	2:A:526:LEU:HA	1.90	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 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	C	145/149 (97%)	138 (95%)	7 (5%)	0	100	100
1	D	145/149 (97%)	138 (95%)	7 (5%)	0	100	100
2	A	578/670 (86%)	532 (92%)	45 (8%)	1 (0%)	52	86
2	B	578/670 (86%)	533 (92%)	44 (8%)	1 (0%)	52	86
All	All	1446/1638 (88%)	1341 (93%)	103 (7%)	2 (0%)	59	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	120	LYS
2	B	120	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	C	126/128 (98%)	126 (100%)	0	100	100
1	D	126/128 (98%)	126 (100%)	0	100	100
2	A	488/586 (83%)	487 (100%)	1 (0%)	95	97
2	B	488/586 (83%)	488 (100%)	0	100	100
All	All	1228/1428 (86%)	1227 (100%)	1 (0%)	95	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	519	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	54	ASN
2	A	465	GLN
2	B	465	GLN
2	B	519	ASN
1	D	42	GLN
1	D	54	ASN

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)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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	$\#\|Z\| > 2$
4	CLR	A	701	-	31,31,31	0.77	1 (3%)	48,48,48	1.37	5 (10%)
4	CLR	B	701	-	31,31,31	0.77	1 (3%)	48,48,48	1.37	5 (10%)

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
4	CLR	A	701	-	-	0/10/68/68	0/4/4/4
4	CLR	B	701	-	-	0/10/68/68	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	CLR	C10-C9	-2.04	1.52	1.56
4	B	701	CLR	C10-C9	-2.02	1.52	1.56

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	701	CLR	C13-C17-C20	-4.20	112.66	119.49
4	A	701	CLR	C13-C17-C20	-4.18	112.69	119.49
4	B	701	CLR	C13-C14-C8	-3.72	108.56	114.36
4	A	701	CLR	C13-C14-C8	-3.71	108.58	114.36
4	A	701	CLR	C11-C12-C13	-2.70	107.96	112.81
4	B	701	CLR	C11-C12-C13	-2.66	108.03	112.81
4	A	701	CLR	C4-C5-C10	2.13	119.50	116.41
4	B	701	CLR	C4-C5-C10	2.17	119.55	116.41
4	B	701	CLR	C17-C13-C14	3.11	103.72	100.09
4	A	701	CLR	C17-C13-C14	3.17	103.79	100.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	CLR	14	0
4	B	701	CLR	15	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.