



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Jul 17, 2017 – 01:35 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.; Mancina, F.
Deposited on : unknown
Resolution : 3.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

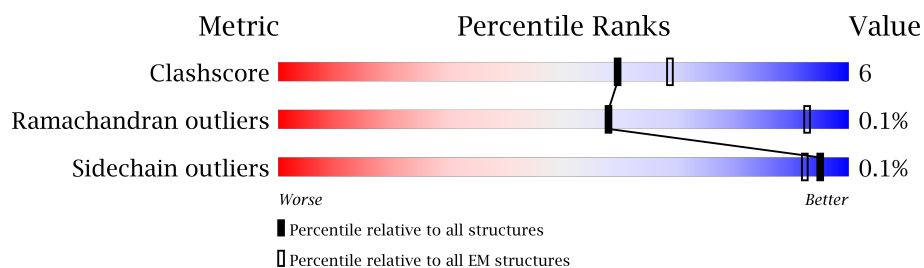
1 Overall quality at a glance

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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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 $\leq 5\%$.

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 [i](#)

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		

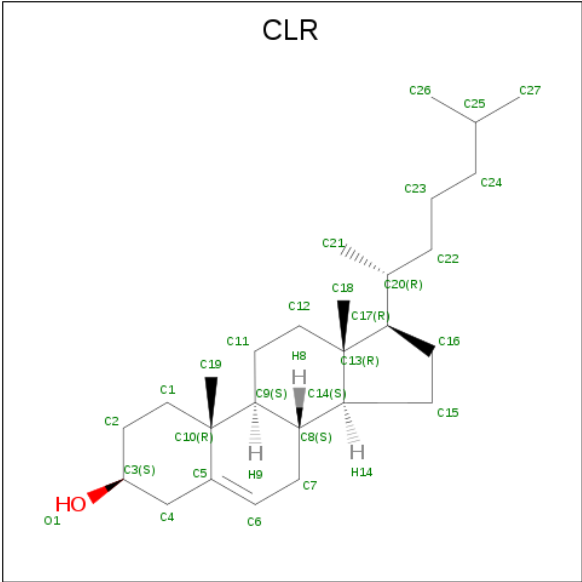
- Molecule 2 is a protein called STRA6.

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: C₂₇H₄₆O).



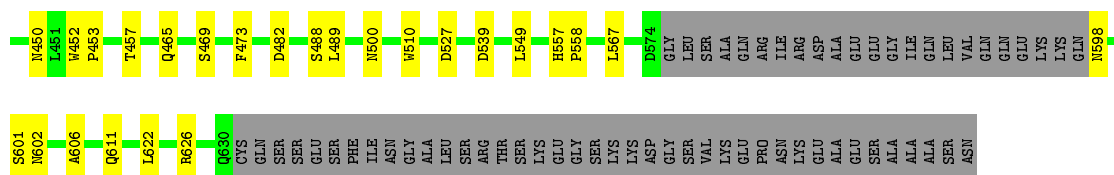
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			28	27	1	
4	B	1	Total	C	O	0
			28	27	1	

- Molecule 1: Calmodulin

MET
 A2
 Q42
 Q50
 D51
 M52
 I53
 N54
 M72
 R75
 E84
 E88
 M110
 E115
 S148
 LYS

Q630	CYS	M450	H145	MET
GLN	L451	Y150	ALA	SER
SER	M452	Q167	GLU	THR
SER	P463	Y178	VAL	ASN
GLU	Q465	Y181	ASP	TYR
SER	S469	G185	TYR	ASP
PHE	F473	Y200	SER	TYR
ASN	D482	L204	ASP	THR
GLY	S488	K234	GLU	GLN
LEU	L489	K235	ASN	ALA
ARG	M500	K236	ALA	ALA
THR	R511	K249	PRO	PRO
SER	R519	L250	THR	THR
GLY	M519	R253	LYS	LYS
LYS	L526	D256	ALA	ALA
GLU	D527	T264	PRO	PRO
GLY	P540	F269	VAL	VAL
SER	L549	L298	E26	E26
VAL	D574	L301	P33	P33
GLU	GLY	A313	D36	D36
PRO	LEU	L316	E37	E37
ASN	SER	M325	F40	F40
LYS	GLU	L363	H41	H41
GLU	ALA	H367	M52	M52
ALA	GLN	L371	S65	S65
SER	ARG	M414	D66	D66
ALA	ILE	L423	R69	R69
ALA	ARG	M598	G70	G70
ALA	ASP	S601	L71	L71
ALA	ALA	G602	T72	T72
ALA	ALA	L606	G73	G73
SER	ALA	LYS	L74	L74
SER	ALA	LYS	L75	L75
ASN	ASN	GLN	H109	H109
		GLN	P112	P112
		GLN	K120	K120
		GLN	T125	T125
		GLN	Y136	Y136
		GLN	P137	P137
		GLN	L138	L138

Y150	Y151	Y152	Y153	Y154	Y155	Y156	Y157	Y158	Y159	Y160	Y161	Y162	Y163	Y164	Y165	Y166	Y167	Y168	Y169	Y170	Y171	Y172	Y173	Y174	Y175	Y176	Y177	Y178	Y179	Y180	Y181	Y182	Y183	Y184	Y185	Y186	Y187	Y188	Y189	Y190	Y191	Y192	Y193	Y194	Y195	Y196	Y197	Y198	Y199	Y200																																																																					
Q167	Q168	Q169	Q170	Q171	Q172	Q173	Q174	Q175	Q176	Q177	Q178	Q179	Q180	Q181	Q182	Q183	Q184	Q185	Q186	Q187	Q188	Q189	Q190	Q191	Q192	Q193	Q194	Q195	Q196	Q197	Q198	Q199	Q200	Q201	Q202	Q203	Q204	Q205	Q206	Q207	Q208	Q209	Q210	Q211	Q212	Q213	Q214	Q215	Q216	Q217	Q218	Q219	Q220																																																																		
Q221	Q222	Q223	Q224	Q225	Q226	Q227	Q228	Q229	Q230	Q231	Q232	Q233	Q234	Q235	Q236	Q237	Q238	Q239	Q240	Q241	Q242	Q243	Q244	Q245	Q246	Q247	Q248	Q249	Q250	Q251	Q252	Q253	Q254	Q255	Q256	Q257	Q258	Q259	Q260	Q261	Q262	Q263	Q264	Q265	Q266	Q267	Q268	Q269	Q270	Q271	Q272	Q273	Q274	Q275	Q276	Q277	Q278	Q279	Q280																																																												
Q281	Q282	Q283	Q284	Q285	Q286	Q287	Q288	Q289	Q290	Q291	Q292	Q293	Q294	Q295	Q296	Q297	Q298	Q299	Q300	Q301	Q302	Q303	Q304	Q305	Q306	Q307	Q308	Q309	Q310	Q311	Q312	Q313	Q314	Q315	Q316	Q317	Q318	Q319	Q320	Q321	Q322	Q323	Q324	Q325	Q326	Q327	Q328	Q329	Q330	Q331	Q332	Q333	Q334	Q335	Q336	Q337	Q338	Q339	Q340	Q341	Q342	Q343	Q344	Q345	Q346	Q347	Q348	Q349	Q350	Q351	Q352	Q353	Q354	Q355	Q356	Q357	Q358	Q359	Q360	Q361	Q362	Q363	Q364	Q365	Q366	Q367	Q368	Q369	Q370	Q371	Q372	Q373	Q374	Q375	Q376	Q377	Q378	Q379	Q380	Q381	Q382	Q383	Q384	Q385	Q386	Q387	Q388	Q389	Q390	Q391	Q392	Q393	Q394	Q395	Q396	Q397	Q398	Q399	Q400
Q401	Q402	Q403	Q404	Q405	Q406	Q407	Q408	Q409	Q410	Q411	Q412	Q413	Q414	Q415	Q416	Q417	Q418	Q419	Q420	Q421	Q422	Q423	Q424	Q425	Q426	Q427	Q428	Q429	Q430	Q431	Q432	Q433	Q434	Q435	Q436	Q437	Q438	Q439	Q440	Q441	Q442	Q443	Q444	Q445	Q446	Q447	Q448	Q449	Q450	Q451	Q452	Q453	Q454	Q455	Q456	Q457	Q458	Q459	Q460	Q461	Q462	Q463	Q464	Q465	Q466	Q467	Q468	Q469	Q470	Q471	Q472	Q473	Q474	Q475	Q476	Q477	Q478	Q479	Q480	Q481	Q482	Q483	Q484	Q485	Q486	Q487	Q488	Q489	Q490	Q491	Q492	Q493	Q494	Q495	Q496	Q497	Q498	Q499	Q500																				
Q501	Q502	Q503	Q504	Q505	Q506	Q507	Q508	Q509	Q510	Q511	Q512	Q513	Q514	Q515	Q516	Q517	Q518	Q519	Q520	Q521	Q522	Q523	Q524	Q525	Q526	Q527	Q528	Q529	Q530	Q531	Q532	Q533	Q534	Q535	Q536	Q537	Q538	Q539	Q540	Q541	Q542	Q543	Q544	Q545	Q546	Q547	Q548	Q549	Q550	Q551	Q552	Q553	Q554	Q555	Q556	Q557	Q558	Q559	Q560	Q561	Q562	Q563	Q564	Q565	Q566	Q567	Q5																																																				



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	56615	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	100	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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%)	51	84
2	B	578/670 (86%)	533 (92%)	44 (8%)	1 (0%)	51	84
All	All	1446/1638 (88%)	1341 (93%)	103 (7%)	2 (0%)	58	88

All (2) Ramachandran outliers are listed below:

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

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	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%)	94	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 ⓘ

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 ⓘ

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	0.79	1 (3%)	48,48,48	1.41	6 (12%)
4	CLR	B	701	-	31,31,31	0.79	1 (3%)	48,48,48	1.41	6 (12%)

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	-2.10	1.52	1.56
4	B	701	CLR	C10-C9	-2.09	1.52	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	CLR	C13-C17-C20	-4.24	112.66	119.47
4	A	701	CLR	C13-C17-C20	-4.22	112.69	119.47
4	B	701	CLR	C13-C14-C8	-3.82	108.56	114.39
4	A	701	CLR	C13-C14-C8	-3.81	108.58	114.39
4	A	701	CLR	C11-C12-C13	-2.78	107.96	112.80
4	B	701	CLR	C11-C12-C13	-2.74	108.03	112.80
4	A	701	CLR	C7-C8-C9	2.00	112.24	109.72
4	B	701	CLR	C7-C8-C9	2.10	112.36	109.72
4	A	701	CLR	C4-C5-C10	2.25	119.50	116.41
4	B	701	CLR	C4-C5-C10	2.29	119.55	116.41
4	B	701	CLR	C17-C13-C14	3.06	103.72	100.07
4	A	701	CLR	C17-C13-C14	3.11	103.79	100.07

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.