



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:48 PM GMT

PDB ID : 2W2C
Title : STRUCTURE OF THE TETRADECAMERIC OLIGOMERISATION DOMAIN OF CALCIUM-CALMODULIN DEPENDENT PROTEIN KINASE II DELTA
Authors : Pike, A.C.W.; Rellos, P.; Sethi, R.; Salah, E.; Burgess-Brown, N.; Shrestha, L.; Roos, A.; Murray, J.W.; Von Delft, F.; Edwards, A.; Arrowsmith, C.H.; Weigelt, J.; Bountra, C.; Knapp, S.
Deposited on : 2008-10-28
Resolution : 2.70 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

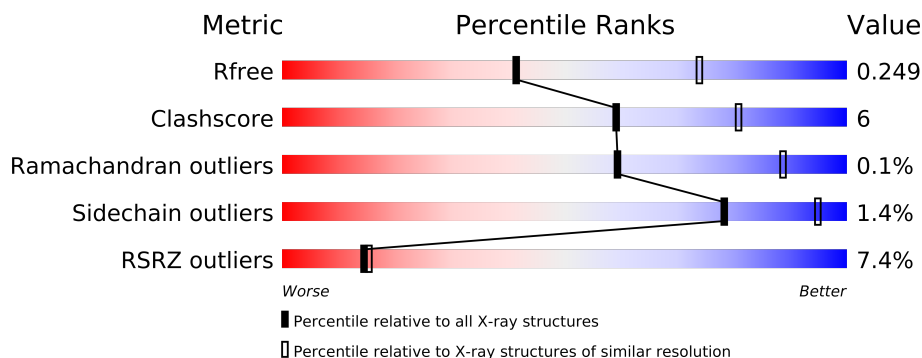
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	144	
1	B	144	
1	C	144	
1	D	144	
1	E	144	
1	F	144	
1	G	144	
1	H	144	
1	I	144	
1	J	144	
1	K	144	
1	L	144	
1	M	144	
1	N	144	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	B	632	-	X
2	ACT	C	632	-	X
2	ACT	D	632	-	X
2	ACT	E	632	-	X
2	ACT	I	632	-	X
2	ACT	K	632	-	X
2	ACT	L	632	-	X
2	ACT	M	632	-	X
2	ACT	N	632	-	X
3	CD	B	1472	-	X

2 Entry composition

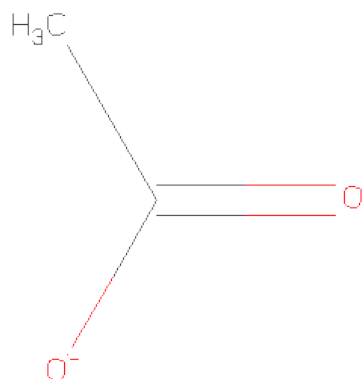
There are 4 unique types of molecules in this entry. The entry contains 14067 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			996	630	174	186	6			
1	B	128	Total	C	N	O	S	0	0	0
			1011	640	175	190	6			
1	C	127	Total	C	N	O	S	0	0	0
			992	628	174	184	6			
1	D	125	Total	C	N	O	S	0	0	0
			988	626	173	183	6			
1	E	129	Total	C	N	O	S	0	0	0
			994	627	175	187	5			
1	F	126	Total	C	N	O	S	0	0	0
			986	623	173	184	6			
1	G	127	Total	C	N	O	S	0	0	0
			991	625	175	186	5			
1	H	131	Total	C	N	O	S	0	0	0
			1010	636	178	191	5			
1	I	128	Total	C	N	O	S	0	0	0
			985	625	171	184	5			
1	J	125	Total	C	N	O	S	0	0	0
			972	617	168	181	6			
1	K	127	Total	C	N	O	S	0	0	0
			983	624	174	179	6			
1	L	130	Total	C	N	O	S	0	0	0
			1014	640	177	191	6			
1	M	125	Total	C	N	O	S	0	0	0
			975	620	171	179	5			
1	N	131	Total	C	N	O	S	0	0	0
			1015	644	175	190	6			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		
2	I	1	Total	C	O	0	0
			4	2	2		
2	J	1	Total	C	O	0	0
			4	2	2		
2	K	1	Total	C	O	0	0
			4	2	2		
2	L	1	Total	C	O	0	0
			4	2	2		
2	M	1	Total	C	O	0	0
			4	2	2		
2	N	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total 1	Cd 1	0	0
3	B	1	Total 1	Cd 1	0	0
3	J	3	Total 3	Cd 3	0	0
3	F	1	Total 1	Cd 1	0	0

- Molecule 4 is water.

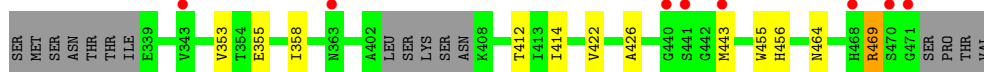
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	10	Total 10	O 10	0	0
4	C	5	Total 5	O 5	0	0
4	D	8	Total 8	O 8	0	0
4	E	5	Total 5	O 5	0	0
4	F	5	Total 5	O 5	0	0
4	G	9	Total 9	O 9	0	0
4	H	6	Total 6	O 6	0	0
4	I	9	Total 9	O 9	0	0
4	J	8	Total 8	O 8	0	0
4	K	4	Total 4	O 4	0	0
4	L	5	Total 5	O 5	0	0
4	M	4	Total 4	O 4	0	0
4	N	8	Total 8	O 8	0	0

3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

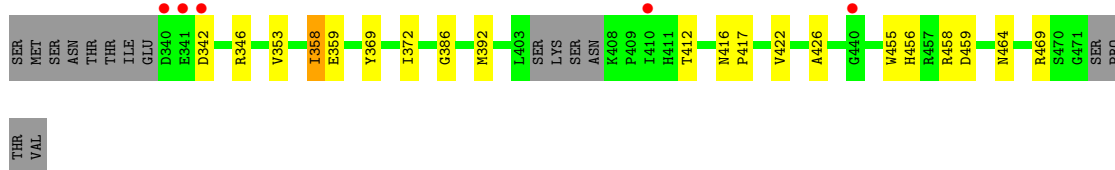
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain A: 



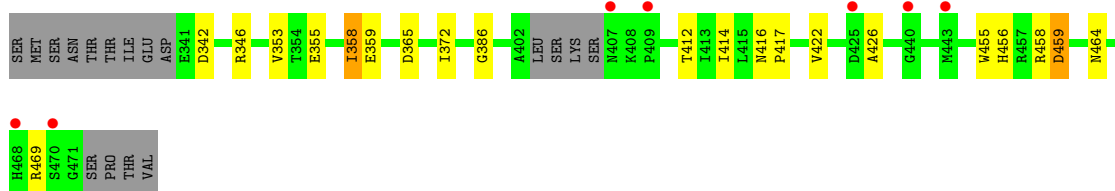
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain B: 



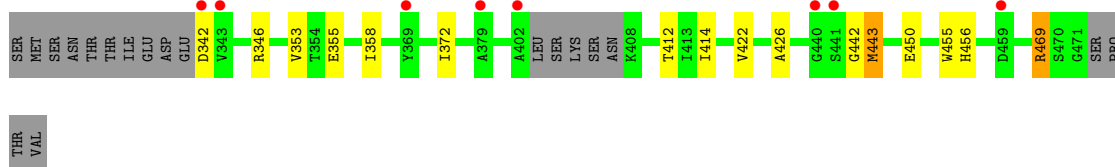
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain C: 



- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain D: 



- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain E: 



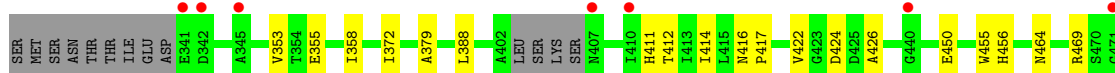
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain F: 



- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain G: 



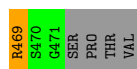
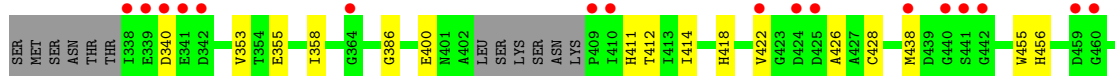
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain H: 



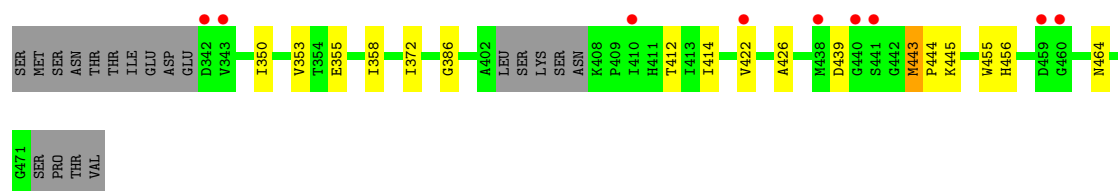
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain I: 



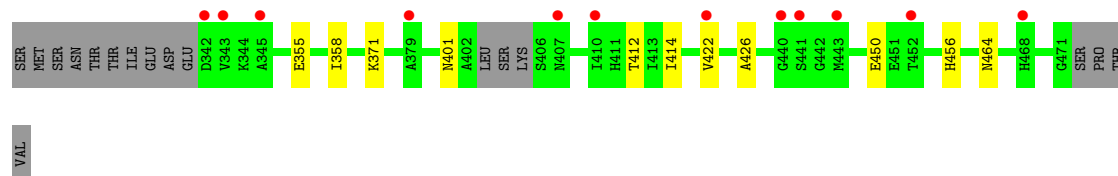
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain J: 



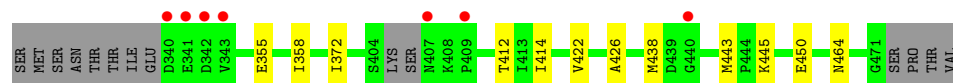
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain K:



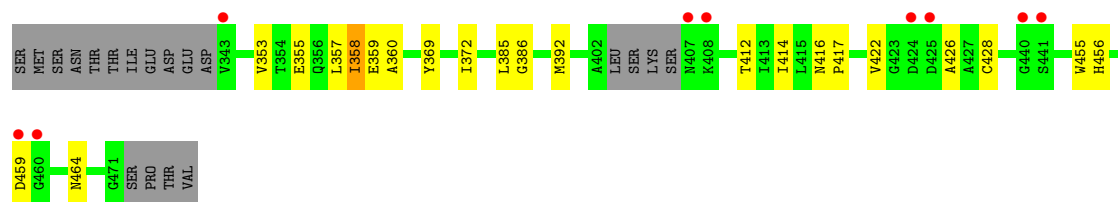
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain L:



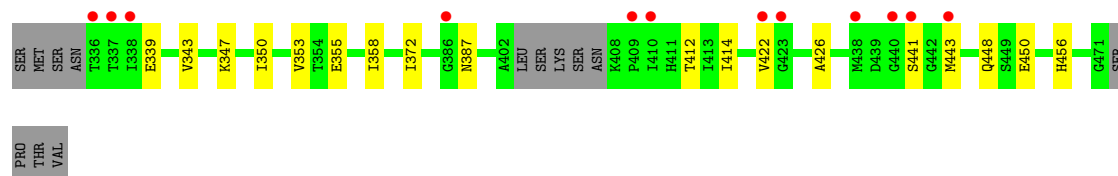
- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain M:



- Molecule 1: CALCIUM/CALMODULIN-DEPENDENTPROTEIN KINASE TYPE II DELTA CHAIN

Chain N:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.55Å 117.80Å 160.76Å 90.00° 111.92° 90.00°	Depositor
Resolution (Å)	44.80 – 2.70 43.37 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.80-2.70) 99.5 (43.37-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0055	Depositor
R, R_{free}	0.211 , 0.245 0.219 , 0.249	Depositor DCC
R_{free} test set	2134 reflections (3.11%)	DCC
Wilson B-factor (Å ²)	70.9	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 20.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 70678 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14067	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.75	0/1020	0.72	2/1385 (0.1%)
1	B	0.85	0/1035	0.76	1/1403 (0.1%)
1	C	0.73	0/1016	0.77	2/1380 (0.1%)
1	D	0.77	0/1012	0.76	2/1372 (0.1%)
1	E	0.66	0/1018	0.72	0/1386
1	F	0.66	0/1010	0.72	1/1371 (0.1%)
1	G	0.69	0/1015	0.71	0/1379
1	H	0.64	0/1034	0.70	1/1407 (0.1%)
1	I	0.67	1/1009 (0.1%)	0.69	1/1372 (0.1%)
1	J	0.65	0/996	0.71	0/1354
1	K	0.67	1/1007 (0.1%)	0.73	0/1368
1	L	0.75	0/1038	0.72	0/1409
1	M	0.75	1/999 (0.1%)	0.73	0/1357
1	N	0.67	0/1039	0.72	0/1412
All	All	0.71	3/14248 (0.0%)	0.73	10/19355 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	428	CYS	CB-SG	-7.37	1.69	1.82
1	I	428	CYS	CB-SG	-5.22	1.73	1.81
1	K	450	GLU	CG-CD	5.12	1.59	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	469	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	469	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	H	469	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	D	469	ARG	NE-CZ-NH2	5.54	123.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	469	ARG	NE-CZ-NH2	5.37	122.99	120.30
1	F	469	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	C	469	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	A	469	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	D	443	MET	CG-SD-CE	5.05	108.29	100.20
1	A	469	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	996	0	903	12	0
1	B	1011	0	931	16	0
1	C	992	0	908	16	1
1	D	988	0	920	20	0
1	E	994	0	893	12	0
1	F	986	0	902	13	0
1	G	991	0	901	18	0
1	H	1010	0	908	16	1
1	I	985	0	889	15	1
1	J	972	0	887	15	0
1	K	983	0	903	10	1
1	L	1014	0	926	15	0
1	M	975	0	895	16	0
1	N	1015	0	928	17	0
2	A	4	0	3	1	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	1	0
2	E	4	0	3	0	0
2	F	4	0	3	0	0
2	G	4	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	4	0	3	1	0
2	I	4	0	3	1	0
2	J	4	0	3	0	0
2	K	4	0	3	0	0
2	L	4	0	3	0	0
2	M	4	0	3	0	0
2	N	4	0	3	0	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	3	0	0	0	0
4	A	7	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	D	8	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	2	0
4	G	9	0	0	0	0
4	H	6	0	0	0	0
4	I	9	0	0	3	0
4	J	8	0	0	0	0
4	K	4	0	0	0	0
4	L	5	0	0	0	0
4	M	4	0	0	0	0
4	N	8	0	0	0	0
All	All	14067	0	12736	163	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (163) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:443:MET:HE2	1:D:443:MET:HA	1.31	1.12
1:G:411:HIS:CE1	4:I:2003:HOH:O	2.23	0.91
1:B:422:VAL:HG12	1:L:426:ALA:HB2	1.62	0.81
1:G:411:HIS:HE1	4:I:2003:HOH:O	1.62	0.81
1:N:441:SER:O	1:N:443:MET:HE2	1.85	0.76
1:D:443:MET:CE	1:D:443:MET:HA	2.12	0.75
1:J:443:MET:HE3	1:J:444:PRO:HD2	1.66	0.75
1:A:422:VAL:HG12	1:K:426:ALA:HB2	1.68	0.74
1:J:439:ASP:HB3	1:J:445:LYS:CD	2.18	0.73
1:B:422:VAL:HG12	1:L:426:ALA:CB	2.20	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:422:VAL:HG13	1:H:456:HIS:HB2	1.74	0.69
1:D:442:GLY:O	1:D:443:MET:CE	2.43	0.66
1:C:422:VAL:HG12	1:D:426:ALA:HB2	1.78	0.65
1:E:456:HIS:HB2	1:H:422:VAL:HG13	1.77	0.65
1:B:426:ALA:HB2	1:L:422:VAL:HG12	1.81	0.63
1:B:359:GLU:OE1	1:B:359:GLU:HA	1.99	0.62
1:A:426:ALA:HB2	1:K:422:VAL:HG12	1.80	0.62
1:F:426:ALA:HB2	1:J:422:VAL:HG12	1.82	0.62
1:I:426:ALA:HB2	1:N:422:VAL:HG12	1.82	0.61
1:A:422:VAL:HG12	1:K:426:ALA:CB	2.30	0.61
1:D:442:GLY:O	1:D:443:MET:HE3	2.00	0.60
1:I:456:HIS:HB2	1:N:422:VAL:HG13	1.85	0.59
1:I:422:VAL:HG12	1:N:426:ALA:HB2	1.84	0.59
1:D:358:ILE:HG21	1:D:412:THR:HG21	1.85	0.58
1:A:358:ILE:HG21	1:A:412:THR:HG21	1.85	0.58
1:C:456:HIS:HB2	1:D:422:VAL:HG13	1.86	0.57
1:C:422:VAL:HG12	1:D:426:ALA:CB	2.35	0.57
1:H:358:ILE:HG21	1:H:412:THR:HG21	1.87	0.57
1:E:422:VAL:HG12	1:H:426:ALA:HB2	1.87	0.57
1:A:355:GLU:HG2	1:A:414:ILE:HD12	1.86	0.57
1:F:418:HIS:NE2	4:F:2002:HOH:O	2.33	0.57
1:I:469:ARG:HH12	2:I:632:ACT:H3	1.69	0.57
1:A:456:HIS:HB2	1:K:422:VAL:HG13	1.86	0.56
1:G:358:ILE:HG21	1:G:412:THR:HG21	1.88	0.56
1:F:355:GLU:HG2	1:F:414:ILE:HD12	1.87	0.56
1:G:426:ALA:HB2	1:M:422:VAL:HG12	1.87	0.56
1:L:355:GLU:HG2	1:L:414:ILE:HD12	1.88	0.56
1:B:353:VAL:HG13	1:B:455:TRP:CZ2	2.41	0.56
1:A:355:GLU:CG	1:A:414:ILE:HD12	2.37	0.55
1:F:422:VAL:HG12	1:J:426:ALA:HB2	1.87	0.55
1:L:443:MET:CE	1:L:445:LYS:NZ	2.70	0.55
1:D:443:MET:CA	1:D:443:MET:HE2	2.22	0.54
1:M:359:GLU:HA	1:M:359:GLU:OE1	2.07	0.54
1:B:369:TYR:CD2	1:B:392:MET:HE1	2.43	0.54
1:D:442:GLY:O	1:D:443:MET:HE2	2.08	0.54
1:C:422:VAL:HG13	1:D:456:HIS:HB2	1.89	0.54
1:N:339:GLU:O	1:N:343:VAL:HG23	2.08	0.53
1:F:456:HIS:HB2	1:J:422:VAL:HG13	1.89	0.53
1:K:358:ILE:HG21	1:K:412:THR:HG21	1.91	0.53
1:F:422:VAL:HG13	1:J:456:HIS:HB2	1.91	0.53
1:C:359:GLU:OE1	1:C:359:GLU:HA	2.08	0.53
1:A:422:VAL:HG13	1:K:456:HIS:HB2	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:422:VAL:HG13	1:N:456:HIS:HB2	1.90	0.52
1:D:469:ARG:NH1	2:D:632:ACT:OXT	2.42	0.52
1:H:393:ASP:CG	1:I:411:HIS:HE2	2.12	0.52
1:C:358:ILE:HG21	1:C:412:THR:HG21	1.91	0.52
1:H:355:GLU:HG2	1:H:414:ILE:HD12	1.91	0.52
1:C:426:ALA:HB2	1:D:422:VAL:HG12	1.92	0.52
1:G:422:VAL:HG13	1:M:456:HIS:HB2	1.92	0.52
1:B:358:ILE:HG21	1:B:412:THR:HG21	1.92	0.52
1:B:342:ASP:OD1	1:B:346:ARG:HD2	2.09	0.51
1:F:355:GLU:CG	1:F:414:ILE:HD12	2.40	0.51
1:N:355:GLU:HG2	1:N:414:ILE:HD12	1.91	0.51
1:L:355:GLU:CG	1:L:414:ILE:HD12	2.41	0.51
1:E:358:ILE:HG21	1:E:412:THR:HG21	1.93	0.51
1:B:422:VAL:O	1:L:426:ALA:HB2	2.10	0.51
1:C:353:VAL:HG13	1:C:455:TRP:CZ2	2.46	0.51
1:E:415:LEU:HD21	1:N:387:ASN:HB3	1.93	0.50
1:H:339:GLU:O	1:H:343:VAL:HG23	2.11	0.50
1:J:358:ILE:HG21	1:J:412:THR:HG21	1.93	0.50
1:G:456:HIS:HB2	1:M:422:VAL:HG13	1.94	0.49
1:J:355:GLU:HG2	1:J:414:ILE:HD12	1.93	0.49
1:M:353:VAL:HG13	1:M:455:TRP:CZ2	2.47	0.49
1:N:372:ILE:O	1:N:372:ILE:HG22	2.12	0.49
1:K:355:GLU:HG2	1:K:414:ILE:HD12	1.94	0.49
1:D:372:ILE:O	1:D:372:ILE:HG22	2.13	0.49
1:I:355:GLU:HG2	1:I:414:ILE:HD12	1.94	0.49
1:N:355:GLU:CG	1:N:414:ILE:HD12	2.43	0.49
1:G:372:ILE:O	1:G:372:ILE:HG22	2.14	0.48
1:B:372:ILE:O	1:B:372:ILE:HG22	2.13	0.48
1:C:386:GLY:HA2	1:D:450:GLU:OE2	2.13	0.48
1:E:355:GLU:HG2	1:E:414:ILE:HD12	1.94	0.48
1:B:353:VAL:HG13	1:B:455:TRP:CH2	2.49	0.48
1:I:355:GLU:CG	1:I:414:ILE:HD12	2.44	0.48
1:L:443:MET:HE1	1:L:445:LYS:NZ	2.29	0.48
1:C:458:ARG:O	1:C:459:ASP:C	2.52	0.48
1:F:358:ILE:HG21	1:F:412:THR:HG21	1.96	0.48
1:H:355:GLU:CG	1:H:414:ILE:HD12	2.44	0.48
1:K:355:GLU:CG	1:K:414:ILE:HD12	2.44	0.47
1:D:355:GLU:HG2	1:D:414:ILE:HD12	1.95	0.47
1:G:422:VAL:HG12	1:M:426:ALA:HB2	1.96	0.47
1:I:358:ILE:HG21	1:I:412:THR:HG21	1.96	0.47
1:A:426:ALA:CB	1:K:422:VAL:HG12	2.44	0.47
1:J:355:GLU:CG	1:J:414:ILE:HD12	2.45	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:355:GLU:HG3	1:C:414:ILE:HD12	1.97	0.47
1:B:342:ASP:O	1:B:346:ARG:HG3	2.15	0.47
1:H:404:SER:O	1:H:407:ASN:N	2.48	0.46
1:L:443:MET:CE	1:L:445:LYS:HZ3	2.27	0.46
1:N:358:ILE:HG21	1:N:412:THR:HG21	1.96	0.46
1:E:408:LYS:CB	1:E:409:PRO:HD2	2.45	0.46
1:B:456:HIS:HB2	1:L:422:VAL:HG13	1.97	0.46
1:M:369:TYR:CD2	1:M:392:MET:HE1	2.51	0.46
1:G:426:ALA:CB	1:M:422:VAL:HG12	2.45	0.46
1:D:355:GLU:CG	1:D:414:ILE:HD12	2.45	0.46
1:H:469:ARG:HH12	2:H:632:ACT:H3	1.81	0.46
1:D:342:ASP:OD1	1:D:346:ARG:HG3	2.15	0.46
1:F:426:ALA:CB	1:J:422:VAL:HG12	2.46	0.46
1:J:372:ILE:O	1:J:372:ILE:HG22	2.15	0.46
1:I:426:ALA:CB	1:N:422:VAL:HG12	2.46	0.45
1:I:418:HIS:NE2	4:I:2007:HOH:O	2.36	0.45
1:E:372:ILE:HG22	1:E:372:ILE:O	2.16	0.45
1:M:355:GLU:HG3	1:M:414:ILE:HD12	1.98	0.45
1:D:443:MET:CA	1:D:443:MET:CE	2.91	0.45
1:M:358:ILE:HG21	1:M:412:THR:HG21	1.98	0.45
1:L:443:MET:HE2	1:L:445:LYS:NZ	2.32	0.44
1:M:353:VAL:HG13	1:M:455:TRP:CH2	2.52	0.44
1:E:355:GLU:CG	1:E:414:ILE:HD12	2.48	0.44
1:H:353:VAL:HG13	1:H:455:TRP:CZ2	2.52	0.44
1:G:355:GLU:HG2	1:G:414:ILE:HD12	2.00	0.44
1:H:401:ASN:HB3	1:I:438:MET:SD	2.57	0.44
1:B:386:GLY:HA2	1:L:450:GLU:OE2	2.18	0.44
1:I:386:GLY:HA2	1:N:450:GLU:OE2	2.18	0.43
1:G:469:ARG:NH1	2:G:632:ACT:OXT	2.51	0.43
1:H:353:VAL:HG13	1:H:455:TRP:CH2	2.53	0.43
1:G:355:GLU:CG	1:G:414:ILE:HD12	2.49	0.43
1:F:422:VAL:HG12	1:J:426:ALA:CB	2.49	0.43
1:N:350:ILE:O	1:N:353:VAL:HG12	2.18	0.43
1:C:422:VAL:O	1:C:426:ALA:HB3	2.19	0.43
1:F:420:HIS:ND1	4:F:2003:HOH:O	2.12	0.43
1:E:386:GLY:HA2	1:H:450:GLU:OE2	2.18	0.43
1:M:357:LEU:O	1:M:360:ALA:HB3	2.18	0.42
1:B:458:ARG:O	1:B:459:ASP:C	2.58	0.42
1:L:358:ILE:HG21	1:L:412:THR:HG21	2.01	0.42
1:C:416:ASN:N	1:C:417:PRO:CD	2.83	0.42
1:L:372:ILE:O	1:L:372:ILE:HG22	2.19	0.42
1:F:353:VAL:HG13	1:F:455:TRP:CZ2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:353:VAL:HG13	1:J:455:TRP:CZ2	2.55	0.42
1:M:372:ILE:HG22	1:M:372:ILE:O	2.20	0.42
1:C:372:ILE:O	1:C:372:ILE:HG22	2.20	0.41
1:I:422:VAL:HG12	1:N:426:ALA:CB	2.49	0.41
1:J:350:ILE:O	1:J:353:VAL:HG12	2.20	0.41
1:A:469:ARG:HH12	2:A:632:ACT:H3	1.84	0.41
1:C:342:ASP:O	1:C:346:ARG:HG3	2.20	0.41
1:G:353:VAL:HG13	1:G:455:TRP:CZ2	2.55	0.41
1:G:353:VAL:HG13	1:G:455:TRP:CH2	2.55	0.41
1:M:385:LEU:HB3	1:N:448:GLN:NE2	2.36	0.41
1:A:422:VAL:O	1:A:426:ALA:HB3	2.20	0.41
1:G:424:ASP:N	1:G:424:ASP:OD1	2.52	0.41
1:C:353:VAL:HG13	1:C:455:TRP:CH2	2.55	0.41
1:N:343:VAL:CG1	1:N:347:LYS:HE3	2.50	0.41
1:M:416:ASN:N	1:M:417:PRO:CD	2.83	0.41
1:B:416:ASN:N	1:B:417:PRO:CD	2.84	0.41
1:D:353:VAL:HG13	1:D:455:TRP:CZ2	2.56	0.41
1:E:450:GLU:OE2	1:H:386:GLY:HA2	2.21	0.41
1:I:353:VAL:HG13	1:I:455:TRP:CZ2	2.56	0.41
1:E:353:VAL:HG13	1:E:455:TRP:CZ2	2.56	0.40
1:H:343:VAL:HG12	1:H:347:LYS:HE3	2.03	0.40
1:A:353:VAL:HG13	1:A:455:TRP:CH2	2.55	0.40
1:G:416:ASN:N	1:G:417:PRO:CD	2.85	0.40
1:G:450:GLU:OE2	1:M:386:GLY:HA2	2.21	0.40
1:G:379:ALA:O	1:G:388:LEU:HD12	2.21	0.40
1:K:401:ASN:HB3	1:L:438:MET:SD	2.61	0.40
1:F:450:GLU:OE2	1:J:386:GLY:HA2	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:365:ASP:OD2	1:H:359:GLU:OE2[3_445]	2.11	0.09
1:I:400:GLU:O	1:K:371:LYS:NZ[3_545]	2.19	0.01

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 X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone

conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	124/144 (86%)	120 (97%)	4 (3%)	0	100	100
1	B	124/144 (86%)	119 (96%)	5 (4%)	0	100	100
1	C	123/144 (85%)	119 (97%)	3 (2%)	1 (1%)	27	58
1	D	121/144 (84%)	118 (98%)	3 (2%)	0	100	100
1	E	125/144 (87%)	123 (98%)	2 (2%)	0	100	100
1	F	122/144 (85%)	117 (96%)	5 (4%)	0	100	100
1	G	123/144 (85%)	119 (97%)	4 (3%)	0	100	100
1	H	127/144 (88%)	123 (97%)	4 (3%)	0	100	100
1	I	124/144 (86%)	119 (96%)	5 (4%)	0	100	100
1	J	121/144 (84%)	118 (98%)	3 (2%)	0	100	100
1	K	123/144 (85%)	118 (96%)	5 (4%)	0	100	100
1	L	126/144 (88%)	120 (95%)	6 (5%)	0	100	100
1	M	121/144 (84%)	116 (96%)	4 (3%)	1 (1%)	27	58
1	N	127/144 (88%)	123 (97%)	4 (3%)	0	100	100
All	All	1731/2016 (86%)	1672 (97%)	57 (3%)	2 (0%)	59	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	459	ASP
1	C	459	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	97/126 (77%)	95 (98%)	2 (2%)	66	91
1	B	101/126 (80%)	99 (98%)	2 (2%)	68	92
1	C	98/126 (78%)	96 (98%)	2 (2%)	68	92
1	D	100/126 (79%)	100 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	97/126 (77%)	96 (99%)	1 (1%)	85	97
1	F	98/126 (78%)	97 (99%)	1 (1%)	85	97
1	G	98/126 (78%)	97 (99%)	1 (1%)	85	97
1	H	99/126 (79%)	96 (97%)	3 (3%)	53	84
1	I	95/126 (75%)	94 (99%)	1 (1%)	84	96
1	J	96/126 (76%)	94 (98%)	2 (2%)	66	91
1	K	96/126 (76%)	95 (99%)	1 (1%)	85	97
1	L	101/126 (80%)	100 (99%)	1 (1%)	85	97
1	M	95/126 (75%)	93 (98%)	2 (2%)	66	91
1	N	100/126 (79%)	100 (100%)	0	100	100
All	All	1371/1764 (78%)	1352 (99%)	19 (1%)	78	95

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	MET
1	A	464	ASN
1	B	358	ILE
1	B	464	ASN
1	C	358	ILE
1	C	464	ASN
1	E	464	ASN
1	F	464	ASN
1	G	464	ASN
1	H	404	SER
1	H	407	ASN
1	H	464	ASN
1	I	340	ASP
1	J	443	MET
1	J	464	ASN
1	K	464	ASN
1	L	464	ASN
1	M	358	ILE
1	M	464	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	387	ASN
1	G	411	HIS
1	H	387	ASN
1	H	407	ASN
1	I	448	GLN
1	M	387	ASN
1	M	448	GLN
1	N	448	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\# Z > 2$
2	ACT	A	632	-	1,3,3	2.47	1 (100%)	0,3,3	0.00	-
2	ACT	B	632	-	1,3,3	5.07	1 (100%)	0,3,3	0.00	-
2	ACT	C	632	-	1,3,3	4.63	1 (100%)	0,3,3	0.00	-
2	ACT	D	632	-	1,3,3	4.61	1 (100%)	0,3,3	0.00	-
2	ACT	E	632	-	1,3,3	3.15	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	F	632	-	1,3,3	2.00	1 (100%)	0,3,3	0.00	-
2	ACT	G	632	-	1,3,3	3.39	1 (100%)	0,3,3	0.00	-
2	ACT	H	632	-	1,3,3	4.89	1 (100%)	0,3,3	0.00	-
2	ACT	I	632	-	1,3,3	3.76	1 (100%)	0,3,3	0.00	-
2	ACT	J	632	-	1,3,3	4.34	1 (100%)	0,3,3	0.00	-
2	ACT	K	632	-	1,3,3	5.09	1 (100%)	0,3,3	0.00	-
2	ACT	L	632	-	1,3,3	4.01	1 (100%)	0,3,3	0.00	-
2	ACT	M	632	-	1,3,3	3.33	1 (100%)	0,3,3	0.00	-
2	ACT	N	632	-	1,3,3	2.25	1 (100%)	0,3,3	0.00	-

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	ACT	A	632	-	-	0/0/0/0	0/0/0/0
2	ACT	B	632	-	-	0/0/0/0	0/0/0/0
2	ACT	C	632	-	-	0/0/0/0	0/0/0/0
2	ACT	D	632	-	-	0/0/0/0	0/0/0/0
2	ACT	E	632	-	-	0/0/0/0	0/0/0/0
2	ACT	F	632	-	-	0/0/0/0	0/0/0/0
2	ACT	G	632	-	-	0/0/0/0	0/0/0/0
2	ACT	H	632	-	-	0/0/0/0	0/0/0/0
2	ACT	I	632	-	-	0/0/0/0	0/0/0/0
2	ACT	J	632	-	-	0/0/0/0	0/0/0/0
2	ACT	K	632	-	-	0/0/0/0	0/0/0/0
2	ACT	L	632	-	-	0/0/0/0	0/0/0/0
2	ACT	M	632	-	-	0/0/0/0	0/0/0/0
2	ACT	N	632	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	632	ACT	CH3-C	5.09	1.56	1.48
2	B	632	ACT	CH3-C	5.07	1.56	1.48
2	H	632	ACT	CH3-C	4.89	1.55	1.48
2	C	632	ACT	CH3-C	4.63	1.55	1.48
2	D	632	ACT	CH3-C	4.61	1.55	1.48
2	J	632	ACT	CH3-C	4.34	1.55	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	632	ACT	CH3-C	4.01	1.54	1.48
2	I	632	ACT	CH3-C	3.76	1.54	1.48
2	G	632	ACT	CH3-C	3.39	1.53	1.48
2	M	632	ACT	CH3-C	3.33	1.53	1.48
2	E	632	ACT	CH3-C	3.15	1.53	1.48
2	A	632	ACT	CH3-C	2.47	1.52	1.48
2	N	632	ACT	CH3-C	2.25	1.52	1.48
2	F	632	ACT	CH3-C	2.00	1.51	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	128/144 (88%)	0.62	8 (6%) 19 21	36, 42, 52, 55	0
1	B	128/144 (88%)	0.45	5 (3%) 37 42	34, 41, 52, 66	0
1	C	127/144 (88%)	0.49	7 (5%) 24 26	33, 41, 50, 58	0
1	D	125/144 (86%)	0.65	8 (6%) 19 21	36, 42, 51, 55	0
1	E	129/144 (89%)	0.60	8 (6%) 20 22	38, 45, 52, 56	0
1	F	126/144 (87%)	0.53	10 (7%) 13 13	40, 45, 52, 56	0
1	G	127/144 (88%)	0.47	7 (5%) 24 26	38, 44, 52, 55	0
1	H	131/144 (90%)	0.62	13 (9%) 8 8	36, 44, 52, 59	0
1	I	128/144 (88%)	0.81	17 (13%) 4 4	37, 44, 52, 54	0
1	J	125/144 (86%)	0.51	9 (7%) 15 16	39, 45, 51, 53	0
1	K	127/144 (88%)	0.63	12 (9%) 9 8	35, 42, 51, 54	0
1	L	130/144 (90%)	0.69	7 (5%) 25 27	35, 42, 52, 57	0
1	M	125/144 (86%)	0.50	9 (7%) 15 16	36, 43, 51, 57	0
1	N	131/144 (90%)	0.67	12 (9%) 9 9	38, 45, 51, 55	0
All	All	1787/2016 (88%)	0.59	132 (7%) 14 15	33, 44, 52, 66	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	336	THR	6.6
1	G	341	GLU	6.1
1	E	441	SER	6.0
1	M	459	ASP	5.5
1	L	340	ASP	5.4
1	H	422	VAL	5.3
1	F	341	GLU	5.2
1	K	443	MET	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	459	ASP	4.9
1	L	343	VAL	4.8
1	D	342	ASP	4.6
1	M	407	ASN	4.4
1	I	338	ILE	4.2
1	D	343	VAL	4.2
1	J	441	SER	4.1
1	B	340	ASP	4.0
1	E	338	ILE	4.0
1	A	440	GLY	4.0
1	E	440	GLY	4.0
1	F	402	ALA	3.9
1	K	342	ASP	3.9
1	K	441	SER	3.9
1	J	343	VAL	3.9
1	I	440	GLY	3.8
1	N	423	GLY	3.8
1	F	440	GLY	3.8
1	G	342	ASP	3.7
1	D	440	GLY	3.7
1	N	422	VAL	3.6
1	H	440	GLY	3.5
1	G	440	GLY	3.5
1	I	342	ASP	3.5
1	L	440	GLY	3.4
1	C	440	GLY	3.3
1	K	407	ASN	3.3
1	I	341	GLU	3.3
1	B	341	GLU	3.3
1	H	441	SER	3.3
1	H	421	LEU	3.2
1	I	459	ASP	3.2
1	I	442	GLY	3.2
1	D	459	ASP	3.2
1	N	438	MET	3.1
1	I	409	PRO	3.1
1	A	443	MET	3.1
1	J	438	MET	3.0
1	N	440	GLY	3.0
1	G	407	ASN	3.0
1	G	345	ALA	2.9
1	B	440	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	426	ALA	2.9
1	I	410	ILE	2.8
1	I	422	VAL	2.8
1	J	460	GLY	2.8
1	N	441	SER	2.8
1	J	342	ASP	2.7
1	E	402	ALA	2.7
1	J	410	ILE	2.7
1	L	409	PRO	2.7
1	E	459	ASP	2.7
1	F	422	VAL	2.7
1	I	364	GLY	2.7
1	I	460	GLY	2.7
1	J	440	GLY	2.7
1	K	440	GLY	2.7
1	D	402	ALA	2.7
1	F	410	ILE	2.7
1	L	342	ASP	2.6
1	N	338	ILE	2.6
1	H	343	VAL	2.6
1	I	441	SER	2.6
1	A	343	VAL	2.5
1	K	410	ILE	2.5
1	D	441	SER	2.4
1	N	443	MET	2.4
1	B	342	ASP	2.4
1	C	470	SER	2.4
1	I	339	GLU	2.4
1	H	459	ASP	2.4
1	I	340	ASP	2.4
1	A	471	GLY	2.4
1	I	425	ASP	2.4
1	G	410	ILE	2.4
1	D	369	TYR	2.4
1	N	337	THR	2.4
1	M	460	GLY	2.3
1	H	407	ASN	2.3
1	H	439	ASP	2.3
1	K	422	VAL	2.3
1	N	409	PRO	2.3
1	H	427	ALA	2.3
1	C	409	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	422	VAL	2.3
1	N	410	ILE	2.3
1	C	407	ASN	2.3
1	K	379	ALA	2.3
1	D	379	ALA	2.3
1	H	397	PHE	2.3
1	E	442	GLY	2.3
1	M	425	ASP	2.2
1	K	468	HIS	2.2
1	M	440	GLY	2.2
1	I	438	MET	2.2
1	I	424	ASP	2.2
1	F	441	SER	2.2
1	C	468	HIS	2.2
1	F	343	VAL	2.2
1	K	343	VAL	2.2
1	M	424	ASP	2.2
1	E	443	MET	2.2
1	B	410	ILE	2.2
1	H	340	ASP	2.2
1	A	468	HIS	2.1
1	K	452	THR	2.1
1	C	443	MET	2.1
1	A	470	SER	2.1
1	M	441	SER	2.1
1	K	345	ALA	2.1
1	L	407	ASN	2.1
1	M	408	LYS	2.1
1	N	386	GLY	2.1
1	J	459	ASP	2.1
1	E	339	GLU	2.1
1	H	442	GLY	2.1
1	M	343	VAL	2.1
1	A	363	ASN	2.1
1	A	441	SER	2.1
1	C	425	ASP	2.1
1	F	421	LEU	2.1
1	G	471	GLY	2.1
1	F	408	LYS	2.0
1	L	341	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ACT	M	632	4/4	0.35	4.65	67,67,68,68	0
3	CD	B	1472	1/1	0.31	4.41	82,82,82,82	1
2	ACT	L	632	4/4	0.29	4.07	56,57,57,58	0
2	ACT	K	632	4/4	0.42	3.65	45,48,48,48	0
2	ACT	C	632	4/4	0.41	3.31	55,58,58,58	0
2	ACT	D	632	4/4	0.39	2.82	52,55,55,55	0
2	ACT	E	632	4/4	0.35	2.65	63,65,65,65	0
2	ACT	I	632	4/4	0.32	2.60	65,67,67,68	0
2	ACT	N	632	4/4	0.31	2.29	74,76,76,76	0
2	ACT	B	632	4/4	0.28	2.26	48,51,51,51	0
2	ACT	J	632	4/4	0.26	1.50	60,62,62,62	0
2	ACT	H	632	4/4	0.27	1.36	54,56,56,57	0
3	CD	H	1472	1/1	0.33	1.24	78,78,78,78	1
2	ACT	A	632	4/4	0.31	1.05	50,51,52,53	0
2	ACT	G	632	4/4	0.25	0.69	58,58,59,59	0
3	CD	J	1474	1/1	0.27	0.30	94,94,94,94	1
2	ACT	F	632	4/4	0.20	-0.03	67,68,68,68	0
3	CD	F	1472	1/1	0.17	-0.80	96,96,96,96	1
3	CD	J	1472	1/1	0.23	-0.85	79,79,79,79	1
3	CD	J	1473	1/1	0.19	-1.18	77,77,77,77	1

6.5 Other polymers ⓘ

There are no such residues in this entry.