



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:52 AM UTC

PDB ID : 2VQA / pdb_00002vqa
Title : Protein-folding location can regulate Mn versus Cu- or Zn-binding. Crystal Structure of MncA.
Authors : Tottey, S.; Waldron, K.J.; Firbank, S.J.; Reale, B.; Bessant, C.; Sato, K.; Gray, J.; Banfield, M.J.; Dennison, C.; Robinson, N.J.
Deposited on : 2008-03-12
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

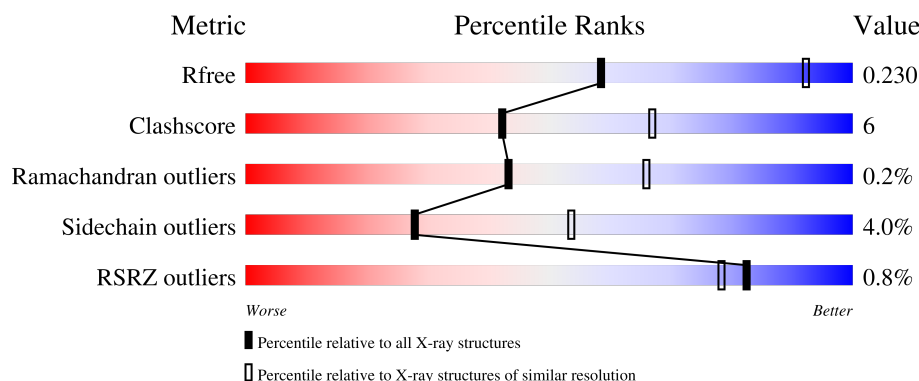
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

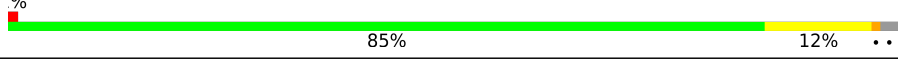
The reported resolution of this entry is 2.95 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	361	
1	B	361	
1	C	361	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	1395	-	-	X	-
3	ACT	B	1395	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SLL1358 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2748	1764	461	517	6			
1	B	356	Total	C	N	O	S	0	0	0
			2752	1766	461	519	6			
1	C	354	Total	C	N	O	S	0	0	0
			2736	1756	458	516	6			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

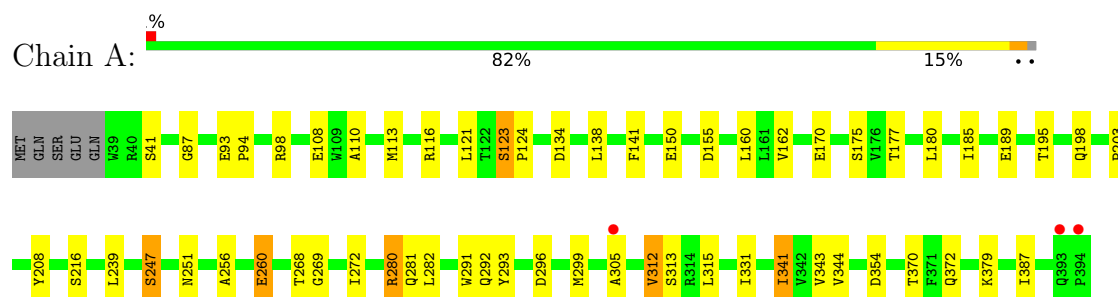
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	8	Total O 8 8	0	0
4	C	10	Total O 10 10	0	0

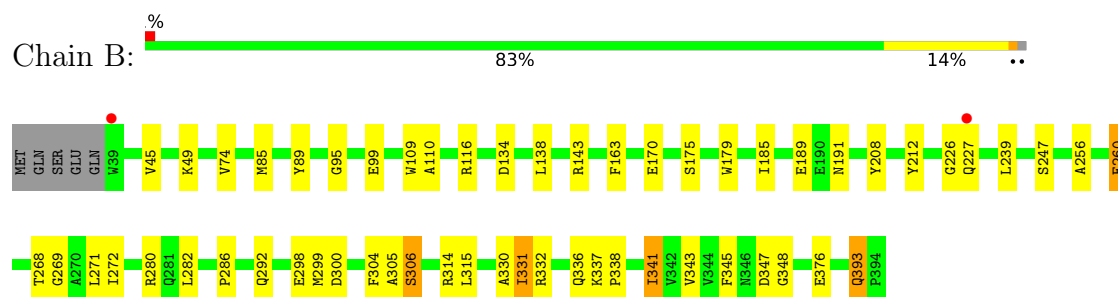
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

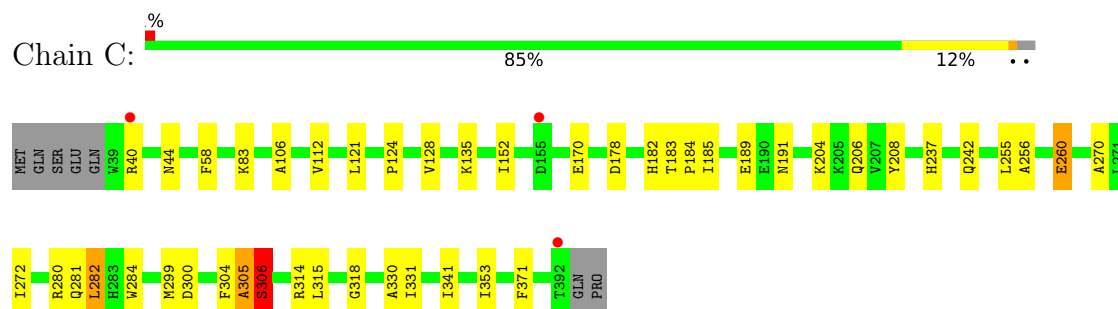
• Molecule 1: SLL1358 PROTEIN



• Molecule 1: SLL1358 PROTEIN



• Molecule 1: SLL1358 PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	236.19Å 236.19Å 134.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	58.32 – 2.95 58.32 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (58.32-2.95) 100.0 (58.32-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.02 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.233 0.193 , 0.230	Depositor DCC
R_{free} test set	2386 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 7.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8306	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MN, 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	0.65	0/2831	0.90	4/3867 (0.1%)
1	B	0.69	1/2835 (0.0%)	0.89	0/3872
1	C	0.71	3/2818 (0.1%)	0.90	1/3848 (0.0%)
All	All	0.68	4/8484 (0.0%)	0.90	5/11587 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	305	ALA	CA-CB	-7.19	1.44	1.54
1	C	304	PHE	C-O	-7.03	1.15	1.24
1	C	306	SER	C-O	-6.37	1.16	1.24
1	B	304	PHE	C-O	-6.03	1.17	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	305	ALA	N-CA-C	-6.06	100.33	109.79
1	A	123	SER	CA-C-N	5.19	126.33	119.84
1	A	123	SER	C-N-CA	5.19	126.33	119.84
1	C	106	ALA	N-CA-C	5.09	116.79	108.55
1	A	312	VAL	N-CA-C	-5.02	101.64	108.06

There are no chirality outliers.

There are no planarity outliers.

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	2748	0	2661	37	0
1	B	2752	0	2665	45	0
1	C	2736	0	2650	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	8	0	6	2	0
3	B	12	0	9	3	0
3	C	12	0	9	1	0
4	A	14	0	0	0	0
4	B	8	0	0	1	0
4	C	10	0	0	1	0
All	All	8306	0	8000	103	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 (103) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:ALA:O	1:B:306:SER:HB3	1.49	1.06
1:C:170:GLU:HG2	1:C:208:TYR:OH	1.56	1.05
1:B:170:GLU:HG2	1:B:208:TYR:OH	1.71	0.91
1:C:272:ILE:HD11	3:C:1393:ACT:H1	1.57	0.86
1:A:170:GLU:HG2	1:A:208:TYR:OH	1.76	0.86
1:A:299:MET:HE3	1:A:315:LEU:HD13	1.61	0.81
1:C:282:LEU:HD13	1:C:330:ALA:HB2	1.68	0.76
1:B:305:ALA:O	1:B:306:SER:CB	2.30	0.75
1:B:393:GLN:NE2	1:B:393:GLN:HA	2.00	0.75
1:B:170:GLU:CG	1:B:208:TYR:OH	2.35	0.74
1:C:282:LEU:CD1	1:C:330:ALA:HB2	2.22	0.69
1:C:300:ASP:OD1	1:C:314:ARG:HG2	1.94	0.68
1:A:185:ILE:O	1:A:189:GLU:HG3	1.94	0.68
1:C:170:GLU:HG2	1:C:208:TYR:HH	1.62	0.65
1:A:292:GLN:HG2	1:A:343:VAL:HG12	1.81	0.63
1:C:305:ALA:O	1:C:306:SER:HB3	1.96	0.63
1:C:305:ALA:O	1:C:306:SER:CB	2.48	0.62
1:B:337:LYS:HB3	1:B:338:PRO:CD	2.30	0.61
1:A:116:ARG:HG2	1:A:134:ASP:OD1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ILE:HD11	3:B:1395:ACT:H3	1.86	0.57
1:B:185:ILE:O	1:B:189:GLU:HG3	2.04	0.57
1:B:282:LEU:HD23	1:B:330:ALA:HB2	1.87	0.57
1:B:116:ARG:HG2	1:B:134:ASP:OD1	2.06	0.56
1:A:195:THR:OG1	1:A:198:GLN:HG3	2.06	0.55
1:B:393:GLN:HA	1:B:393:GLN:HE21	1.71	0.55
1:B:299:MET:HE2	1:B:315:LEU:HD22	1.87	0.55
1:B:299:MET:HE2	1:B:315:LEU:HD13	1.88	0.55
1:B:337:LYS:HB3	1:B:338:PRO:HD3	1.88	0.54
1:B:393:GLN:HE21	1:B:393:GLN:CA	2.19	0.54
1:C:282:LEU:HD13	1:C:330:ALA:CB	2.36	0.54
1:C:255:LEU:HD12	1:C:270:ALA:HB2	1.91	0.52
1:C:183:THR:HG22	1:C:184:PRO:HD2	1.92	0.52
1:C:237:HIS:NE2	1:C:242:GLN:NE2	2.54	0.52
1:B:393:GLN:NE2	1:B:393:GLN:CA	2.65	0.51
1:A:370:THR:HG23	1:B:99:GLU:HB2	1.92	0.51
1:B:85:MET:HA	1:B:163:PHE:O	2.11	0.51
1:A:93:GLU:HB3	1:A:94:PRO:CD	2.41	0.50
1:B:331:ILE:HD11	1:B:341:ILE:HD11	1.93	0.50
1:A:110:ALA:O	1:A:138:LEU:HA	2.11	0.50
1:A:272:ILE:HD12	1:A:341:ILE:HD11	1.93	0.49
1:B:109:TRP:CZ2	1:B:269:GLY:HA3	2.48	0.49
1:A:113:MET:SD	1:A:160:LEU:HD13	2.53	0.49
1:A:299:MET:CE	1:A:315:LEU:HD13	2.40	0.49
1:C:256:ALA:HA	1:C:260:GLU:HG2	1.96	0.48
1:B:239:LEU:HD13	1:B:256:ALA:HB2	1.97	0.47
1:B:337:LYS:CB	1:B:338:PRO:CD	2.93	0.47
1:C:185:ILE:HG22	1:C:189:GLU:OE2	2.14	0.47
1:B:110:ALA:O	1:B:138:LEU:HA	2.15	0.47
1:C:178:ASP:HB2	1:C:206:GLN:HB2	1.96	0.46
1:A:123:SER:HB2	1:A:124:PRO:HD2	1.97	0.46
1:A:41:SER:HA	1:B:185:ILE:HG13	1.96	0.46
1:A:272:ILE:HD11	3:A:1395:ACT:H3	1.97	0.46
1:C:256:ALA:HA	1:C:260:GLU:CG	2.46	0.46
1:C:281:GLN:HB3	4:C:2008:HOH:O	2.15	0.46
1:A:281:GLN:HG3	1:A:387:ILE:O	2.16	0.46
1:A:180:LEU:HD12	1:C:371:PHE:CE1	2.51	0.46
1:C:282:LEU:CD1	1:C:330:ALA:CB	2.92	0.45
1:B:256:ALA:HA	1:B:260:GLU:CG	2.47	0.45
1:C:284:TRP:CZ2	1:C:353:ILE:HD12	2.52	0.45
1:B:272:ILE:HD11	3:B:1395:ACT:CH3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:OE1	1:A:216:SER:OG	2.32	0.45
1:B:239:LEU:HG	1:B:271:LEU:HD12	2.00	0.44
1:A:108:GLU:HB3	1:A:141:PHE:HB2	1.99	0.44
1:A:113:MET:SD	1:A:160:LEU:CD1	3.05	0.44
1:A:162:VAL:HG21	1:A:344:VAL:HG21	1.99	0.44
1:A:268:THR:HG22	1:A:269:GLY:N	2.31	0.44
1:B:292:GLN:HG2	1:B:343:VAL:HG12	1.99	0.44
1:A:312:VAL:O	1:A:313:SER:HB3	2.18	0.44
1:A:121:LEU:HD13	1:A:141:PHE:CD1	2.52	0.43
1:B:45:VAL:HB	1:C:182:HIS:CD2	2.53	0.43
1:B:226:GLY:O	1:B:227:GLN:C	2.60	0.43
1:C:183:THR:CG2	1:C:184:PRO:HD2	2.48	0.43
1:A:256:ALA:O	1:A:268:THR:HG23	2.19	0.43
1:B:143:ARG:HG3	4:B:2002:HOH:O	2.18	0.43
1:C:121:LEU:O	1:C:128:VAL:HA	2.18	0.43
1:A:280:ARG:NH2	1:A:354:ASP:OD2	2.52	0.43
1:A:247:SER:HA	1:A:251:ASN:O	2.18	0.43
1:C:112:VAL:HG12	1:C:135:LYS:HA	2.01	0.43
1:B:286:PRO:HG2	1:C:124:PRO:HG3	2.00	0.42
1:B:300:ASP:HB2	1:B:332:ARG:O	2.19	0.42
1:A:93:GLU:CB	1:A:94:PRO:CD	2.97	0.42
1:A:239:LEU:HD13	1:A:256:ALA:HB2	2.01	0.42
1:B:331:ILE:CD1	1:B:341:ILE:HD11	2.50	0.42
1:A:177:THR:HG22	1:A:203:PRO:HG2	2.01	0.42
1:A:256:ALA:HA	1:A:260:GLU:HG2	2.01	0.42
1:B:95:GLY:O	3:B:1397:ACT:O	2.37	0.42
1:C:58:PHE:HB3	1:C:318:GLY:O	2.19	0.42
1:A:87:GLY:HA3	1:A:291:TRP:CZ2	2.55	0.42
1:B:299:MET:CE	1:B:315:LEU:HD13	2.50	0.42
1:A:272:ILE:HD11	3:A:1395:ACT:CH3	2.50	0.42
1:A:282:LEU:HB3	1:B:179:TRP:CZ2	2.55	0.42
1:A:372:GLN:HG2	1:B:212:TYR:HB2	2.02	0.41
1:A:180:LEU:HD12	1:C:371:PHE:HE1	1.84	0.41
1:B:347:ASP:OD1	1:B:348:GLY:N	2.54	0.41
1:B:331:ILE:HD11	1:B:341:ILE:CD1	2.51	0.41
1:B:376:GLU:H	1:B:376:GLU:CD	2.28	0.41
1:B:331:ILE:CD1	1:B:341:ILE:CD1	2.98	0.41
1:B:89:TYR:CD2	1:B:89:TYR:C	2.98	0.41
1:B:256:ALA:HA	1:B:260:GLU:HG2	2.03	0.41
1:C:299:MET:HE3	1:C:315:LEU:HD13	2.03	0.40
1:B:268:THR:HB	1:B:345:PHE:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:HD21	1:A:293:TYR:CG	2.56	0.40
1:C:299:MET:CE	1:C:315:LEU:HD13	2.51	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 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	354/361 (98%)	335 (95%)	19 (5%)	0	100	100
1	B	354/361 (98%)	335 (95%)	18 (5%)	1 (0%)	36	59
1	C	352/361 (98%)	333 (95%)	18 (5%)	1 (0%)	36	59
All	All	1060/1083 (98%)	1003 (95%)	55 (5%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	306	SER
1	C	306	SER

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 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	292/298 (98%)	282 (97%)	10 (3%)	32	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	293/298 (98%)	280 (96%)	13 (4%)	25	51
1	C	291/298 (98%)	279 (96%)	12 (4%)	27	53
All	All	876/894 (98%)	841 (96%)	35 (4%)	28	53

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ARG
1	A	155	ASP
1	A	175	SER
1	A	247	SER
1	A	260	GLU
1	A	280	ARG
1	A	296	ASP
1	A	331	ILE
1	A	341	ILE
1	A	379	LYS
1	B	49	LYS
1	B	74	VAL
1	B	175	SER
1	B	191	ASN
1	B	247	SER
1	B	260	GLU
1	B	280	ARG
1	B	298	GLU
1	B	314	ARG
1	B	331	ILE
1	B	336	GLN
1	B	341	ILE
1	B	393	GLN
1	C	40	ARG
1	C	44	ASN
1	C	83	LYS
1	C	152	ILE
1	C	191	ASN
1	C	204	LYS
1	C	260	GLU
1	C	280	ARG
1	C	282	LEU
1	C	306	SER
1	C	331	ILE

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Mol	Chain	Res	Type
1	C	341	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	B	201	GLN
1	B	225	GLN
1	B	242	GLN
1	B	393	GLN
1	C	201	GLN
1	C	242	GLN
1	C	292	GLN
1	C	316	GLN
1	C	362	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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
3	ACT	B	1396	-	3,3,3	0.92	0	3,3,3	1.63	1 (33%)
3	ACT	C	1394	-	3,3,3	0.98	0	3,3,3	1.66	1 (33%)
3	ACT	C	1395	-	3,3,3	0.89	0	3,3,3	1.92	2 (66%)
3	ACT	C	1393	2	3,3,3	0.65	0	3,3,3	1.33	0
3	ACT	A	1396	-	3,3,3	0.97	0	3,3,3	1.43	0
3	ACT	A	1395	2	3,3,3	0.89	0	3,3,3	1.21	0
3	ACT	B	1397	-	3,3,3	0.93	0	3,3,3	2.00	1 (33%)
3	ACT	B	1395	2	3,3,3	0.84	0	3,3,3	1.33	0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1397	ACT	OXT-C-O	-2.78	111.73	122.03
3	C	1395	ACT	OXT-C-CH3	2.36	124.97	115.05
3	C	1395	ACT	OXT-C-O	-2.32	113.43	122.03
3	C	1394	ACT	OXT-C-O	-2.28	113.56	122.03
3	B	1396	ACT	OXT-C-O	-2.10	114.24	122.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1393	ACT	1	0
3	A	1395	ACT	2	0
3	B	1397	ACT	1	0
3	B	1395	ACT	2	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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	356/361 (98%)	-0.38	3 (0%) 82 78	12, 12, 12, 12	0
1	B	356/361 (98%)	-0.40	2 (0%) 85 82	12, 12, 12, 12	0
1	C	354/361 (98%)	-0.43	3 (0%) 82 78	12, 12, 12, 12	0
All	All	1066/1083 (98%)	-0.40	8 (0%) 82 78	12, 12, 12, 12	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	PRO	3.5
1	A	393	GLN	3.5
1	C	392	THR	3.5
1	C	155	ASP	2.4
1	A	305	ALA	2.2
1	B	227	GLN	2.2
1	B	39	TRP	2.2
1	C	40	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	C	1394	4/4	0.92	0.17	12,12,12,12	0
3	ACT	C	1395	4/4	0.92	0.14	12,12,12,12	0
3	ACT	A	1396	4/4	0.93	0.20	12,12,12,12	0
3	ACT	B	1396	4/4	0.94	0.13	12,12,12,12	0
3	ACT	B	1397	4/4	0.94	0.12	12,12,12,12	0
3	ACT	C	1393	4/4	0.96	0.11	12,12,12,12	0
3	ACT	B	1395	4/4	0.97	0.08	12,12,12,12	0
2	MN	C	1004	1/1	0.98	0.05	12,12,12,12	0
3	ACT	A	1395	4/4	0.98	0.07	12,12,12,12	0
2	MN	A	1005	1/1	0.98	0.03	12,12,12,12	0
2	MN	B	1001	1/1	0.99	0.04	12,12,12,12	0
2	MN	B	1002	1/1	0.99	0.03	12,12,12,12	0
2	MN	C	1003	1/1	0.99	0.04	12,12,12,12	0
2	MN	A	1006	1/1	0.99	0.03	12,12,12,12	0

6.5 Other polymers

There are no such residues in this entry.